Revised Modeling Protocol for the Beaumont-Port Arthur Area Attainment Demonstration

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1 Summary

This protocol presents the procedures the Texas Commission on Environmental Quality (TCEQ) will use to model ozone and demonstrate attainment of the ozone standard in the Beaumont-Port Arthur (BPA) area using the Comprehensive Air Quality Model with Extensions (CAMx). This modeling will focus on two high ozone episodes, one of which occurred during the 2000 Texas Air Quality Study (TexAQS 2000), and one that occurred just prior to the start of that study. This protocol follows up on the June 2003 Base Case protocol and will focus on photochemical modeling activity up through the base case performance evaluation and then addresses future year inventory development, control strategy testing, and Weight of Evidence analyses.

The objective of this modeling protocol is to enhance the technical credibility of the study by establishing, in advance, agreed-upon procedures for conducting a successful modeling project. Section 2 of the protocol describes the background, objectives, schedule, and organizational structure of the study. The remainder of the protocol describes the following topics: the structure of the modeling system, the development of needed model databases, the plans for meteorological and photochemical model performance evaluation, the future base case inventory development, and the procedures for documenting the base case modeling results.

The current modeling is designed to assess the effectiveness of the control measures adopted in the 1999 and 2000 BPA SIP revisions. Upon completion of this modeling, the TCEQ expects to have demonstrated a strategy that is sufficient to reach attainment. Much of the work for this model application has already been completed in modeling conducted for the adjacent Houston/Galveston/Brazoria (HGB) nonattainment area and is referred to in the past tense. Portions of this study that are new or will be revised during this phase of the modeling are referred to in the future tense.

2 Ozone Modeling Study Design

2.1 Background and Objectives

The 1990 Federal Clean Air Act (FCAA) amendments established five classifications for ozone nonattainment areas based on the magnitude of the monitored 1-hour ozone design values, and established dates by which each classified area should attain the standard. For each nonattainment area, states must develop and submit, to the U.S. Environmental Protection Agency (EPA), a State Implementation Plan (SIP) that demonstrates how the area will attain the standard by the attainment date. EPA designated four ozone nonattainment areas in Texas and classified each. The BPA area was initially designated as a serious ozone nonattainment area,

and was reclassified to moderate in April 1996. Photochemical grid modeling is required to demonstrate attainment.

2.2 2000 BPA Attainment Demonstration

In April 2000, the TNRCC submitted an attainment demonstration to EPA Region VI. This attainment demonstration consisted of the following components:

• Two episodes, August 31- September 2, 1993 and September 8-11, 1993

• Meteorological fields generated by the SAIMM

• Emissions processing using EPS-2 and SMOKE

• Photochemical modeling using CAMx

• Special hourly point source emissions and aerometric data compiled from Coastal Oxidant Assessment for Southeast Texas (COAST) study

TNRCC used modeling to demonstrate that BPA could not attain the 1-hour ozone standard prior to Houston's attainment date of 2007. Therefore, EPA allowed Texas to take advantage of EPA's attainment date extension policy. Using HGB's 2007 attainment date, TNRCC modeled emissions reductions in BPA, with projected control levels in HGB. This modeling, coupled with a weight-of-evidence analysis, demonstrated BPA would achieve attainment of the 1-hour ozone standard by 2007.

EPA approved the BPA attainment demonstration SIP revision in May 2001.

2.3 The TexAQS 2000 Study

From August 15 to September 15, 2000, approximately 250 investigators from more than 35 organizations joined the TNRCC in the TexAQS 2000 field study to carry out research to improve technical understanding of the factors affecting ozone and fine particle concentrations in the eastern half of Texas. TexAQS 2000 was based in Houston, and its work concentrated on the Houston region. TexAQS 2000 collected extensive data useful for supporting photochemical modeling of episodes that occurred during the study period.

2.3.1 Data Collection

The major components of the TexAQS 2000 were the following:

• Six research aircraft, four of which were based in Houston and performed multiple missions:

- The National Oceanic and Atmospheric Administration (NOAA) used a Lockheed Electra as a platform to collect regional chemistry and meteorological measurements to help define regional emissions, chemistry, and transport.

- The Department of Energy provided a Grumman Gulfstream 1 with instrumentation similar to the Electra's to measure both regional and local emission, chemistry, and transport.

- Baylor University operated a Twin Otter for the TNRCC, carrying advanced air quality monitoring instruments similar to those at a Level 2 ground station along with canisters for sampling volatile organic compounds. The Twin Otter's ability to fly slowly made it well-suited to studying urban and industrial plumes.

- NOAA's Environmental Technology Laboratory provided a DC-3 aircraft to measure ozone and fine particles with a downward-looking LIDAR system well-suited to measuring the formation and movement of pollution plumes and to studying the effects of coastal meteorology, including the bay breeze.

- NASA provided two aircraft for use in thermal mapping to help define and evaluate urban and industrial heat-island effects.

- Additional meteorological monitoring to provide data to help describe and understand how wind flows are influenced by bay breezes, sea breezes, and urban and industrial heat islands:

  - Six radar profilers to measure winds and virtual temperature aloft.

  - Two advanced acoustic sounders for the same purpose.

  - Three weather balloon launch sites to measure the temperature and moisture structure of the atmosphere, one of which also had geographic positioning system capability to measure winds aloft.

- A Doppler LIDAR to aid in analysis of the interaction of the bay breeze and the Ship Channel area.

- To the approximately 50 routine, ground-based continuous ozone monitoring sites across the eastern half of Texas and neighboring states, the study added the following:

  - Three Level 2 chemistry monitoring stations to provide detailed, high-sensitivity atmospheric chemistry information on ozone, sulfur dioxide, carbon monoxide, NO, and NO_2.

  - A principal atmospheric chemistry and physics research site at La Porte Airport at which many researchers from universities and national laboratories operated

state-of-the-science instruments to investigate atmospheric processes and measure pollutant concentrations.

- • A smaller advanced research site high on the Williams Tower, about 850 feet above ground level.

- • An hour-by-hour emission inventory of emissions from the Houston and Beaumont/Port Arthur industrial areas, reporting a much more detailed record of emissions than is normally available for either data analysis or photochemical modeling.

2.4 Legal Challenges to 2000 BPA Attainment Demonstration

The US EPA approved the 2000 BPA attainment demonstration SIP in May 2001. As previously noted, this attainment demonstration applied EPA's Attainment Date Extension policy, in which the TNRCC showed that BPA could not attain the 1-hour ozone standard due to ozone and ozone precursor transport from the Houston/Galveston area.   Consequently, EPA allowed BPA to use the same 2007 attainment date as HGB.

In early 2002, EPA's approval of the BPA attainment demonstration was challenged at the Federal 5th Circuit Court of Appeals by a group of petitioners that included the Sierra Club, Clean Air and Water Inc., and Community In-Powerment Development Association. In December 2002, the Circuit Court ruled that EPA did not have the authority to extend attainment dates based on transport from upwind areas. Therefore, BPA, which was designated moderate, did not attain at its statutory deadline of November 15, 1996, which would require bump-up to the next highest category, which is serious. Subsequently, BPA did not attain by that statutory deadline of November 15, 1999.

In early June 2003, EPA proposed two possible paths of action: (1) bump BPA to serious, but have a 2005 attainment date (actually 18 months after bump-up) or (2) bump BPA to severe (either a single double-bump or a second bump-up after finding BPA did not attain in 1999), again with a 2005 attainment date. EPA's bump-up proposal notice went out in June 2003. During roughly the same time frame, EPA proposed implementation guidance for the new 8-hour ozone standard. This proposal includes 8-hour designation schedules. Language in EPA's proposed 8-hour ozone implementation guidance raises the possibility that areas with outstanding 1-hour SIP obligations could transition directly to an 8-hour attainment demonstration. (As of this writing (February 2004), neither the final bump-up notice nor the 8-hour implementation guidance has been signed yet.)

Therefore, TCEQ proposes to go forward with a modeling analysis that meets the 2007 1-hour obligations; a 2005 1-hour analysis that relies on more of a Weight of Evidence approach and a 2010 8-hour modeling analysis that provides for an initial indication of the amount of reductions needed for BPA to meet the 8-hour ozone standard. The timeline will be that of the previously noted 1-hour mid-course review.

2.5 Schedule

Table 1 shows milestones for the photochemical modeling to be conducted under this protocol. Given the caveats on timing noted in the previous paragraph, this schedule is tentative and subject to change.

Table 2-1 - Modeling Milestones and Schedule

Milestones	Date
Development of a Modeling Protocol	June 2003
Development of revised protocol	February 2004
Episode selection and domain specification	May 2002
Meteorological modeling (if needed)	June 2003
Base case emissions inventory preparation (if needed)	June 2003
Base case emission inventory enhancements (to old episodes)	June 2003
Base case performance evaluation	December 2003
Future base inventory development	February 2004
Future base case modeling (including all current controls)	February 2004
Additional control strategy modeling (if needed)	March 2004
Documentation completed	March 2004
Administrative hearing process	April-October 2004
Submittal of Mid Course Review SIP revision to EPA	October 2004

2.6 Modeling/Policy Oversight Groups

2.6.1 Air Quality Advisory Committee

The South East Texas Regional Planning Commission's (SETRPC)Air Quality Advisory Committee (AQAC) serves as the policy oversight group for photochemical modeling, SIP development and other air quality policy issues for the BPA area. Table 2 lists the organizations participating in the work group along with the names of the individuals representing each organization. The members are from a wide variety of organizations affected by the SIP development.

Table 2-2. South East Texas Regional Planning Commission AQAC

Name	Affiliation	Job Title
Mike Magee	TCEQ	BPA SIP Coordinator
Becky Pietras	E.I. DuPont - Orange	Environmental Superintendent

Name	Affiliation	Job Title
Bill Wimberley, Chair	Motiva	
Steve Fitzgibbons	City of Port Arthur	City Manager
Richard Harrel	Lamar University	Professor
Dan W. Deaton	U.S. Department of Energy	
Fred Manhart	Entergy Services, Inc.	Environmental Support Manager - Texas
Paul Reed	ExxonMobil	
Tommy Butts	Bayer	Environmental Division
Bill Forbes	Huntsman Corporation	Manager - Environmental
John Johnson	Jefferson County	Administrative Assistant to County Judge
Lou Fowler	URS Corporation	Program Manager
Martin Novich	Ausimont - USA	Environmental Manager
Morris Carter	Premcor	
Bret Duplant	Unocal	
Michael Leary	Federal Highway Administration	Urban Planner
Nick DeRoos	Beaumont Methanol	Plant Manager
Jennifer DuChamp	Beaumont Methanol	Environmental Coordinator
Georgie Volz	TCEQ-Beaumont	Regional Director
Tom Swulius	Chevron Phillips	Environmental Manager
Earl Geis	Chevron Phillips	Environmental Supervisor
Johnny Casmore, Jr.	Mobil Oil Corporation	Legislative & Regulatory
Ingrid Holmes	City of Beaumont Health Department	Administrator
Chris Rabideau	Shell Global Solutions	
Albert Hendler	URS Corporation	Senior Scientist
Steve Stafford	Texas Department of Transportation	Planning and Programming Engineer
Paula LaRocca	Goodyear Tire & Rubber Company	
Ike Mills	Port Arthur Economic Development Corporation	Deputy Director
Roger Smith	ATOFINA Petro Chemical, Inc.	Environmental Supervisor
Jim Rich	Beaumont Chamber of Commerce	President / CEO
Thomas C. Ho	Lamar University	Professor of Chemical Engineering
Bill Clark	Clark's Pest Control	
Eddie Bates	C & I Oil Company, Inc.	
Candace Broucher	J & R Services	
Ray Hinske	Mobil Chemical-OA/BCSP	Environmental Coordinator
Greg Berwick	Ameripol Synpol Company	EHS Manager
Sid Martinez	Texas Dept of Transportation	Field Representative
Russell Melancon, Jr.	Industrial Safety Training Council	Executive Director
Dennis Isaacs	Dupont Chemical Solutions Enterprise	Environmental Manager
Bob Dickinson	SETRPC	Director of Transportation and Environmental

Name	Affiliation	Job Title
		Resources

2.6.2 Photochemical Modeling Technical Review Committee

The Photochemical Modeling Technical Review Committee has oversight of the technical aspects of applying CAMx to the TexAQS 2000 data. The Photochemical Modeling Technical Review Committee provides review and oversight on the TCEQ photochemical modeling efforts for HGB, as well as BPA. The members of this work group are listed in Table 2-3.

Table 2-3. Photochemical Modeling Technical Review Committee

Name	Company/Organization
Dave Allen	University of Texas at Austin
Ramon Alvarez	Environmental Defense
Dan Baker	Shell Global Solutions
Rob Barrett	Harris County Pollution Control
Harless Benthul	Benthul, Kean, & Woodruff
Pamela Berger	Mayor's Office, City of Houston
Craig Beskid	National Urban Air Toxics Research Center
Daewon Byun	Department of Geophysics, University of Houston
Hsing-wei Chu	Lamar University
Walter Crow	URS Corp.
Alex Cuclis	University of Houston
Mike Cybulski	Clean Air Engineering
Weiping Dai	Trinity Consultants
Stephen Davis	TCEQ
Doug Deason	ExxonMobil Chemical
John Dege	DuPont
Tom Diggs	EPA Region VI
Jon Fisher	Texas Chemical Council
Richard Flannery	TCEQ Region 12
Candace Garrett	TCEQ
Monica R. Gaudet	Metropolitan Transit Authority
Joseph Goldman	CLEAN and ICSEP
Reza Golkarfard	HGAC
Dennis Griffith	Regional Air Quality Planning Commission

K. Hackett	HGAC
John Hall	John Hall Public Affairs
Alan Hansen	Electric Power Research Institute
Albert Hendler	URS Corporation
Elizabeth Hendler	Mid-Course Coalition
T.F. Henken	Baytown
April Hinson	DuPont
David Hitchcock	Houston Advanced Research Center
Thomas C. Ho	Lamar University
Robert E. James	TCEQ Region 12
Steve Kilpatrick	Dow
Alan J. Krol	BP Amoco
John Kush	Reliant Energy
Jane Laping	Mothers for Clean Air
Carole Lenz	Harris County Commissioner Radack, RAQPC, HGAC
Jacqueline Lentz	City of Houston
Jim Lester	Houston Advanced Research Center
Fred Manhart	SETRPC AQAC, Entergy Services, Inc.
Gene McMullen	Bureau of Air Quality Control, City of Houston
Susan Moore	BP Amoco
Quang Nguyen	EPA Region VI
Robert Nolan	ExxonMobil
Bradley Oehler	TCEQ
Barbara Pederson	DuPont
Charles E. Pehl	Pehl Environmental Consulting
Karl Pepple	HGAC
Chris Rabideau	Shell Global Solutions
Rebecca Rentz	Bracewell & Patterson
Dick Robertson	TXU
David Schanbacher	TCEQ
Charles Schleyer	ExxonMobil
George Smith	Sierra Club
Jim Smith	TCEQ
Steve Smith	Lyondell Equistar
Erik Snyder	EPA Region VI
Randall Stowe	Dow

George Talbert	Texas Air Research Center
Tom Tesche	Alpine Geophysics
Don Thompson	TCEQ Region 12
Usha-Marie Turner	TXU
Lilly Wells	HGAC
Mike White	ExxonMobil
Shelley Whitworth	HGAC
John Wilson	GHASP
Jim Yohn	BP Amoco
Steve Ziman	Chevron

2.7 Relation to Other Urban and Regional Modeling Protocols

This protocol (February 2004) includes descriptions of the current CAMx modeling plans for the BPA area, slight changes to the emissions inventory development plans, and procedures for documenting and archiving model results. It is closely related to the latest HGB Mid Course Review modeling protocol (January 2004). Because the TexAQS 2000 study encompasses the HGB ozone nonattainment area in addition to the BPA area, much of the modeling work described in this protocol applies to the HGB area as well.

3 Domain and Database Issues

3.1 Air Quality Data and Meteorological Databases

3.1.1 Surface Measurements

The TCEQ routinely measures meteorological parameters and ozone and concentrations at a number of continuous monitoring sites in Harris, Jefferson, Orange, and Galveston Counties. The City of Houston measures various meteorological parameters and ozone and concentrations at seven sites. Similarly, the South East Texas Regional Planning Commission (SETRPC) maintains a monitoring network that samples for ozone, VOCs (every 12-day cannister samples), and meteorological parameters. In addition, meteorological data are routinely collected at four surface monitors in Victoria County, and two surface monitors in Corpus Christi.

During TexAQS 2000, these routine monitoring networks were complemented by several routine industry-supported networks, including the Houston Regional Monitoring Network, the Texas City/La Marque network, and the SETRPC network. The TCEQ, through the Photochemical Assessment Monitoring Station (PAMS) program, has continuous gas chromatographs to measure

VOC concentrations at three Continuous Air Monitoring Stations (CAMS) in the Houston area (Aldine (CAMS8), Clinton Drive (CAMS403), and Deer Park (CAMS35)). In addition, surface meteorological data and meteorological condition observations are collected at several National Weather Service (NWS) stations in the modeling domain, including Houston Intercontinental Airport. All monitoring performed in the area followed EPA measurement and quality assurance procedures.

3.1.2 Upper Air Measurements

Twice-daily, upper air soundings are taken by the NWS at Corpus Christi, Texas and Lake Charles, Louisiana. These are the upper air monitoring sites closest to the nonattainment area. During TexAQS 2000, this was supplemented by acoustic sounders and radar profilers coupled with radio acoustic sounding systems (RASS), which were used to measure wind direction and velocity at various elevations from 60 meters to 2000 meters. Unfortunately, no radar profiler or sodar data was collected in the BPA area during TexAQS 2000.

3.2 Modeling Episode Selection

This round of modeling is to meet the agency's previous 1-hour mid-course review commitment as well as provide an initial assessment of the new 8-hour ozone standard upon BPA. Experience from previous modeling studies for both BPA and Houston/Galveston indicated that there were substantial advantages in using episodes that occurred during intensive field studies. These are (1) enhanced monitoring and emissions inventory data enables a better analysis of model base case performance, and (2) more confidence can be placed on ozone precursor controls. Consequently, previous modeling studies for the upper Texas Gulf Coast focused on the 1993 COAST study. The TCEQ is currently modeling a set of high ozone days that occurred during TexAQS 2000 for the HGB nonattainment area.

EPA, in its *Guideline for Regulatory Application of the Urban Airshed Model* (*Guideline*), establishes an approach to episode selection that includes identifying meteorological regimes associated with recent high ozone events and ranking them according to the magnitude of the observed ozone. For the 1-hour standard, EPA generally recommended that candidate episodes have monitored ozone greater than 0.120 ppm. Similarly, 8-hour candidate episodes should include monitored ozone values greater than 0.08 ppm. The *Guideline* also acknowledges that data quality and availability are extremely important considerations in episode selection. Previously, the robust, quality-assured COAST data aided the development of reliable wind fields, initial conditions, and boundary conditions. It also provided a large data set of ozone and ozone precursor measurements for evaluating model performance later in the modeling process. The TexAQS 2000 study provides the same types of data and more. Discussions with EPA Region VI led to an abandonment of the previous 1993 COAST episodes, in order to focus on more recent episodes.

In summary, episode selection criteria used were the following:

♦ Episodes that occurred during the TexAQS 2000 study, with its robust data sets.

- BPA episodes that occurred during other (HGB) modeled episodes (potential for transport analyses and conservation of modeling staff resources).
- Episodes that are described by the BPA conceptual model.
- Episodes with relatively high monitored 8-hour ozone (greater than 0.08 ppm).
- Episodes with meteorological regimes (wind flow patterns) representative of high ozone events.
- Closeness of monitored exceedances to 8-hour design values.

Episode selection was made by a team of meteorologists who are familiar with the local and regional meteorological patterns occurring along the Texas Gulf Coast. The TCEQ screened the episodes for monitored ozone greater than 0.120 ppm and attempted to select primary episode days with monitored values approximating the BPA design value of 0.13 ppm.

At least three primary episode days were selected using the criteria listed above and each primary episode day will be preceded by at least one initialization day. When three primary days are part of the same episode, then the initialization day(s) precede only the first of the primary episode days.

3.2.1 Additional Considerations

Due to the large amount of aerometric data collected during TexAQS 2000, episode selection will include consideration of HGB ozone occurrences so that selected episodes may be useful to both nonattainment areas. Since hourly emissions data, as well as ozone and ozone precursor measurements, were collected for both BPA and HGB, it was important to select TexAQS 2000 episode days so that reliable emissions estimates could be generated; thus, ozone predicted using these estimates could be favorably compared to performance evaluation statistics over the entire modeling domain. However, since one of the main findings of TexAQS 2000 was that point source VOC inventories in HGB appear to be underestimated, TCEQ will undertake an analysis to determine if the VOC emissions in BPA are similarly underestimated. This topic is more fully discussed in Section 4 of this protocol.

Although most episodes in the HGB area are multi-day in nature, episodes in BPA are typically a single day/single station in nature. An additional consideration in BPA episode selection is the role of transported ozone and ozone precursors from the HGB area. During TexAQS 2000, there was one multi-day episode in BPA, and multiple stations had exceedances; there was ample evidence of transported pollutants from HGB during this episode.

3.2.2 Beaumont-Port Arthur Conceptual Model

An important component for episode selection is the development of an area-specific conceptual model. Conceptual models are descriptions of the meteorological conditions, air quality values, and emissions data that describe high ozone events for a particular area of interest. A report generated by the University of Texas at Austin and Environ International, *Conceptual Model of Ozone Formation in the Beaumont/Port Arthur Ozone Non-Attainment Area* (October 31, 2002) is Attachment 1 to this protocol.

Follow-up analyses by TCEQ for the BPA conceptual model also includes:

- Flow patterns (source-receptor relationships) for all 8-hour exceedance days from 1998-2002. A complete description of these analyses is Attachment 2 to this protocol.

- Design value trends. The results show that ozone 1-hour design values have been declining, but ozone 8-hour design values have remained constant or increased.

- VOC cannister reactivity - to answer questions of which compounds are most important in the formation of ozone in the BPA areas and whether or not the contribution of certain compound groups to total reactivity has increased or diminished over the last five years.

- Analysis of some Baylor aircraft data.

The additional conceptual model analyses is Attachment 2 to this protocol.

3.2.3 Candidate Episodes

Since TCEQ decided to select high ozone days from among those occurring during TexAQS 2000, the list of available candidate days is narrowed down considerably. Table 3-1 lists the BPA area's exceedances that occurred during TexAQS 2000.

Table 3-1

BPA 1-Hour Ozone Episode Days Occurring During TexAQS 2000

Date	1-hour Ozone Max (ppb)	Monitor Location	Number of hours over 124 ppb
August 30	134	CAMS2 (Beaumont)	1
August 30	133	CAMS9 (West Orange)	1
August 30	165	CAMS28 (Port Arthur West)	2
August 30	131	CAMS64 (Hamshire)	1
August 30	162	CAMS640 (Sabine Pass)	4
August 30	143	CAMS643 (Jefferson County Airport)	2
August 31	152	CAMS640 (Sabine Pass)	2
September 1	160	CAMS28 (Port Arthur West)	2
September 1	144	CAMS64 (Hamshire)	2

| September 1 | 145 | CAMS643 (Jefferson County Airport) | 2 |

August 30-September 1, 2000 is a rare multi-day episode for the BPA area. This time period coincided with a high ozone event in the HGB area as well. In addition, this period is already being modeled by TCEQ for the HGB Mid Course Review SIP, meaning fewer resources would be needed to develop this episode for the BPA attainment demonstration. Analysis of back trajectories indicated that BPA was being affected by transport of ozone and ozone precursors from HGB on all three days.   A search of other BPA exceedance days found that another 1-hour exceedance day occurred on August 12, 2000, just prior to the start of TexAQS 2000. On this day, a 126 ppb maximum was recorded at CAMS28 (Port Arthur West). TCEQ plume sequences indicated that this air parcel went south, over the BPA area, out into the Gulf briefly, and then returned back in with the sea breeze, with the 126 ppb exceedance occurring at 1800 LST. The exceedance does not appear to have any influence from the HGB area and is considered a locally-generated exceedance. Another advantage for using this day is that, even though it does not actually occur during TexAQS 2000, inventories developed for the study period can be easily ported to August 12.

3.2.4 8 - hour Considerations

Table 3-2 lists the high 8-hour ozone values listed for the August 12 and August 30 - September 1, 2000 1-hour episode days. It also includes the "extended" TexAQS 2000 episode (August 19-24 and September 2-6, 2000) Since August 13, 2000 also had 8-hour exceedances, it is included as well.

Table 3-2

8-hour Ozone Exceedances in BPA

Date	8-hour Ozone Max (ppb)	Monitor Location
August 12	99	CAMS28 (Port Arthur West)
August 12	85	CAMS64 (Hamshire)
August 12	88	CAMS640 (Sabine Pass)
August 13	85	CAMS2 (Beaumont)
August 13	89	CAMS64 (Hamshire)
August 19	85	CAMS2 (Beaumont)
August 19	92	CAM9 (West Orange)
August 21	96	CAMS2 (Beaumont)
August 30	88	CAMS2 (Beaumont)
August 30	94	CAMS9 (West Orange)

August 30	115	CAMS28 (Port Arthur West)
August 30	115	CAMS640 (Sabine Pass)
August 30	95	CAMS643 (Jefferson County Airport)
August 31	105	CAMS28 (Port Arthur West)
August 31	85	CAMS64 (Hamshire)
August 31	104	CAMS640 (Sabine Pass)
September 1	87	CAMS9 (West Orange)
September 1	96	CAMS28 (Port Arthur West)
September 1	91	CAMS64 (Hamshire)
September 1	90	CAMS643 (Jefferson County Airport)
September 2	86	CAMS28 (Port Arthur West)
September 4	97	CAMS28 (Port Arthur West)
September 4	97	CAMS640 (Sabine Pass)
September 6	85	CAMS28 (Port Arthur West)

3.2.5 Design Values

A final component used to evaluate the representativeness of an ozone episode day is the comparison of the day's highest monitored ozone to station-specific and area-wide design values. The 8-hour design value is currently defined as the highest 3-year average of each station's 4th-highest 8-hour ozone concentrations (for each of the three years). That is, for each station and each year, a fourth-highest ozone concentration is reported and a three year average for each station is computed. The highest of these averages is the area-wide 8-hour design value. Table 3-3 lists each BPA station's 8-hour design values for 1998-2000, with area-wide design values underlined.

Table 3-3

BPA area design values 1998 - 2000**

Station	8-hour design value (ppb)
CAMS2 (Beaumont)	86
CAMS9 (West Orange)	75
CAMS28 (Port Arthur West)	87
CAMS640 (Sabine Pass)	<u>9</u>5
CAMS642 (Mauriceville)	86
CAMS643 (Jefferson County Airport)	92

** Hamshire (CAMS64) is not included here because 2000 was the first year this station was in operation.

For the 8-hour design values, and using +/- 5 ppb as the criteria for "close" or "preferred", the following days/sites are considered exceedances that are "preferred":

August 13 - 85 ppb at CAMS2 (DV=86)
August 19 - 85 ppb at CAMS2 (86)
August 30 - 88 ppb at CAMS2 (86)
August 30 - 95 ppb at CAMS643 (92)
September 1 - 90 ppb at CAMS643 (92)
September 2 - 86 ppb at CAMS28 (87)
September 4 - 97 ppb at CAMS640 (95)
September 6 - 85 ppb at CAMS28 (87)

If the 8-hour "preferred" definition is relaxed to +/- 10 ppb, this would also include:

August 12 - 88 ppb at CAMS640 (DV=95)
August 21 - 96 ppb at CAMS2 (85)
August 31 - 104 ppb at CAMS640 (95)
September 1 - 96 at CAMS28 (87)
September 4 - 97 ppb at CAMS28 (87)

Therefore, there are a substantial number of exceedances that are close to individual station's design values. For the period August 12-13 and August 19-September 6, 2000, there are 13 "preferred" exceedances and 10 exceedance days.

3.2.6 Selection Procedure

Candidate episode days were evaluated for magnitude of ozone concentration, the number of monitors recording exceedances, the number of hours of exceedance, and closeness to the station's design values. The availability of supplementary aircraft, canister, and continuous gas

chromatograph data was also considered.   Based on the fact that the August 19-September 6, 2000 episode was: (1) a multiday episode; (2) already being modeled for HGB; (3) part of an intensive field campaign; and (4) fit in with the BPA conceptual model, it was chosen as one of the BPA episodes.

The August 12-13, 2000 episode was chosen because (1) it is temporally close to the start of TexAQS 2000 and the August 19-September 6, 2000 episode, therefore the emission inventory data already prepared for the TexAQS 2000 episodes can easily be adjusted for use in the August 12-13, 2000 episode; and (2) within the BPA conceptual model, this is a clear "local" episode.

3.3 Selection of an Air Quality Model

For air quality models to be successfully used as technical support for a regulatory initiative, they must be physically sound. The model performance evaluation described in Section 6 is designed to determine whether the model is a valid tool for identifying potential control strategies. In a regulatory environment it is crucial that oversight groups (e.g., EPA), the regulated community, and the interested public also be convinced of the suitability of the model.

To ensure that a modeling study is defensible, the model must be scientifically appropriate for the intended application and be freely accessible to all stakeholders. The following three simple prerequisites were set for selecting the photochemical grid model to be used for the remainder of the BPA modeling:

1   Must have a reasonably current, peer-reviewed, scientific formulation.

2   Must be available at no or low cost to stakeholders.

3   Must not require the reformatting of available model inputs from any earlier modeling studies.

The only model to meet all three of these criteria is the CAMx. The model is based on well-established treatments of advection, diffusion, deposition, and chemistry. Another important feature is that emissions from large point sources can be treated with the PiG submodel that helps avoid the artificial diffusion that occurs when point source emissions are dumped into a grid volume. The model software and the CAMx user's guide are publicly available at http://www.camx.com. Based upon these selection criteria, the TNRCC committed to using CAMx for SIP modeling in 1999.

It is worth noting that draft EPA guidance for 8-hour ozone modeling attainment demonstrations no longer recommends the use of a specific photochemical grid model. EPA has outlined recommended model selection criteria, which are very similar to the ones the TCEQ used above (peer-reviewed science, available databases, and nonproprietary).

3.4 Modeling Domain and Horizontal Grid Cell Size

The modeling domain for the BPA attainment demonstration is shown in Figure 1. CAMx will also be set up in Lambert Conformal Projection (LCP) because the MM5 meteorological model

uses the LCP coordinate system.   The CAMx projection is defined with the First True Latitude at 30 degrees North, the Second True Latitude at 60 degrees North, and the Central longitude at 100 degrees west. The projection origin is 100 degrees west longitude, 40 degrees north latitude, and the spheroid is a perfect sphere, with a radius of 6370 km. A total of 3 subdomains are employed because CAMx can make use of nested domains. These are described in Table 3-4.

Table 3-4 CAMx Modeling Subdomains

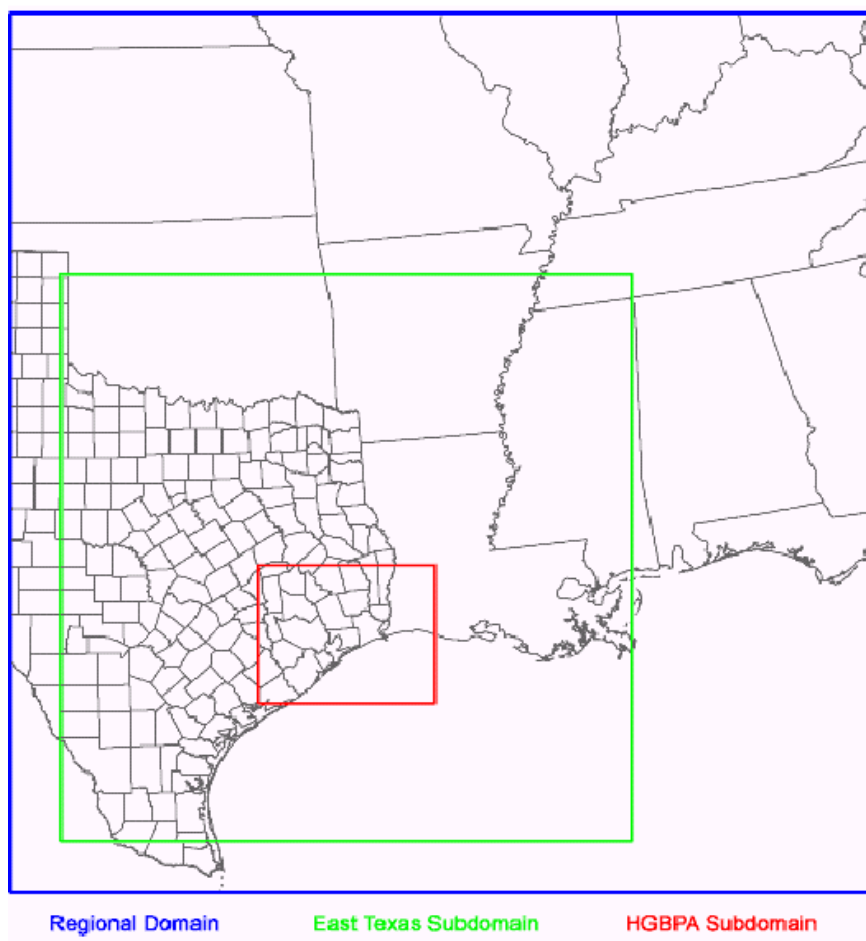| Subdomain	Range		Number of cells		Cell size	
	Easting	Northing	Easting	Northing	Easting	Northing
Regional	(-108,1512)	(-1584,72)	45	46	36	36
East Texas	(-12,1056)	(-1488,-420)	89	89	12	12
HGBBPA	(356,688)	(-1228,-968)	83	65	4	4

Figure 1. The HGBBPA CAMx Modeling Domain

To properly characterize the complex nature of the meteorology on the Gulf Coast, a prognostic meteorological model will be used to develop wind fields. The prognostic model requires a large modeling domain. This large domain also minimizes the impact of boundary conditions within the meteorological model. The meteorological modeling discussion is found in Section 5.

3.5 Number of Vertical Layers

The number of vertical layers is a compromise between including enough detail to accurately characterize the vertical layering of the atmosphere and managing the amount of time required to run the model. Fourteen vertical layers are being used in this study. These layers maintain a constant thickness. The tops of the layers are located at, in sequence: 33.9 meters (m), 84.9 m, 170.5 m, 256.9 m, 343.9 m, 431.7 m, 520.2 m, 609.5 m, 790.5 m, 1068.0 m, 1353.2 m, 2103.0 m, 3025.9 m, and 4105.9 m.

3.6 Model Input Preparation

3.6.1 Wind Field Development

Wind field data included hourly wind direction and wind speed for each three-dimensional grid cell in the domain. For air quality modeling purposes, wind fields are the most important product of the meteorological model. Winds mix pollutants and transport them across the domain. It is critical that the wind fields developed by the meteorological model represent the conditions seen in the actual ozone events, even though it is not reasonable to expect perfect replication. Upper air data may be used to nudge the prognostic wind fields to more closely replicate the observations. A detailed description of the meteorological modeling used to develop the meteorological inputs to CAMx is found in Section 5 of this protocol, Meteorological Modeling.

3.6.2 Mixing Height and Vertical Exchange Coefficients

Mixing height is a useful diagnostic for evaluating the potential impact of emissions and photochemical reactions on air quality. Vertical exchange coefficients (Kv)are typically used in the advection/diffusion equation to calculate mixing between adjacent vertical grid cells. The vertical exchange coefficients required by the photochemical model are calculated in a postprocessing step which imports the model-calculated planetary boundary layer (PBL) height and other predicted variables. These other variables depend on the choice of PBL scheme and may include predicted turbulent kinetic energy (TKE).

3.6.3 Temperature

Prognostic meteorological models, such as MM5, predict hourly temperature values for each grid cell. The surface temperature is one of the variables which forces the growth of the boundary layer, and temperatures aloft are important for the stability of the atmosphere. Emissions of mobile

sources and biogenic sources are temperature dependent, and in the photochemical model the temperatures affect the chemical reaction rates. Model-calculated temperatures may be nudged towards the global analysis fields using Four Dimensional Data Assimilation (FDDA), although surface temperatures are generally not nudged.

3.6.4 Other Meteorological Parameters

Perturbation pressure and the water vapor mixing ratio are prognostic variables which are also passed to a post processing algorithm which calculates five key photolysis rates. The photolysis rates also depend upon the solar zenith angle, altitude, and the spatially and temporally varying albedo, haze, and ozone column information provided by the Total Ozone Monitoring Spectrometric (TOMS) data.

It is necessary to post-process all the meteorological variables described above prior to input into CAMx. Environ (the developers of CAMx) have developed software to convert MM5 outputs to CAMx-ready inputs (MM5CAMX). TCEQ has obtained the necessary software and has used it to convert the MM5 output data.

3.6.5 Initial and Boundary Conditions

The modeling domain was selected to be sufficiently large to help minimize model sensitivity to boundary conditions. In addition, TCEQ will begin modeling two or three days prior to the first
primary day to minimize the sensitivity to initial conditions. Default initial and boundary condition concentrations were used in HGB Phase 1 and in preliminary modeling for the HGB Combined 1-hour and 8-hour Ozone Modeling Analysis (COMA). However, recent modeling analyses conducted in the Dallas/Fort Worth area by Environ showed an unexpectedly large sensitivity of ozone concentrations in that region to the lateral boundary conditions. Consequently, the default ("clean") boundary conditions were replaced by boundary conditions more representative of rural pollutant levels along the regional boundaries. To maintain consistency among modeling applications in Texas, we have adopted the DFW boundary conditions for use in this attainment demonstration. (Sensitivity analyses have shown some improvement in HGB model performance using these somewhat higher concentrations, but the sensitivity to boundary conditions in the HGB region appears to be considerably less than that seen in the DFW modeling.)

As discussed in the DFW modeling final report (available at http://www.tnrcc.state.tx.us/air/aqp/sipmod/dfwaq_techcom.html), the outer edge of the 36 Km. coarse grid was divided into three sections as shown in the figure below (Note that the Dallas/Fort Worth coarse grid is identical to the one we are using for the HGB area). Boundary conditions for each of these segments were set to the values listed in Table 3-5. Initial concentrations were set equal to the values in the last column of the table.
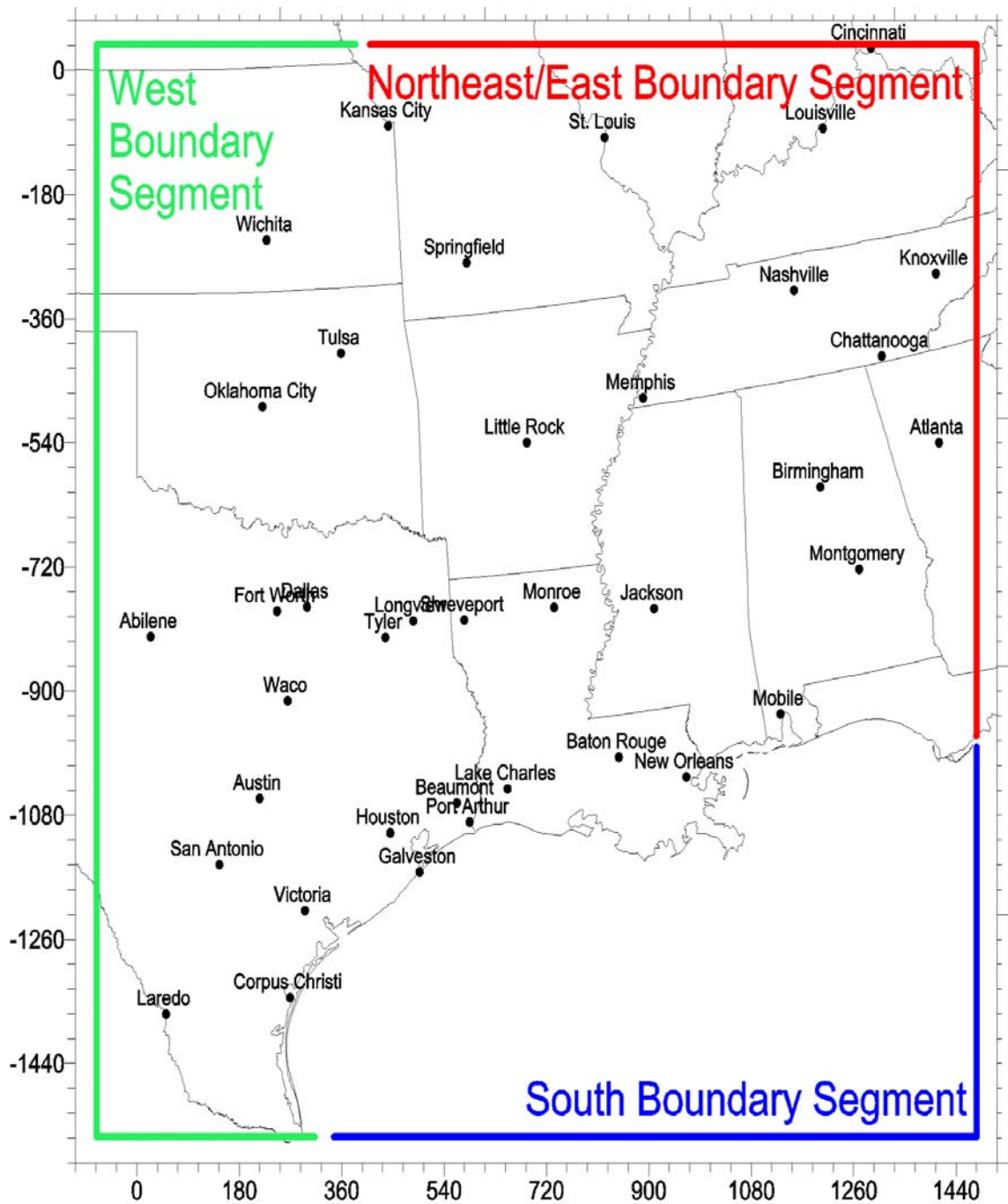
: Segments used to define lateral boundary conditions.

Table 3-5: Boundary Conditions used in HGB COMA

Species	East/Northeastern Boundary Below 1700 m (ppb)	Western Boundary Below 1700 m (ppb)	Southern Boundary and Above 1700 m (ppb)
O3	40.0	40.0	40.0
NO	0.1	0.1	0.1
NO2	1.0	1.0	1.0
CO	200.0	200.0	100.0
PAR	14.9	14.9	14.9
HCHO	2.1	2.1	0.05
ETH	0.51	0.51	0.15
ALD2	0.555	0.555	0.05
TOL	0.18	0.18	0.0786
PAN	0.1	0.1	0.1
HNO2	0.001	0.001	0.001
HNO3	3.0	3.0	1.0
H2O2	3.0	3.0	1.0
OLE	0.3	0.3	0.056
XYL	0.0975	0.0975	0.0688
ISOP	3.6	0.1	0.001
MEOH	8.5	0.001	0.001
ETOH	1.1	0.001	0.001
Total NOx	1.1	1.1	1.1
Total VOC (ppbC)	50.5	22.3	9.3

3.7 Plume-in-Grid Modeling

CAMx has an option to model selected point sources with a PiG algorithm. PiG algorithms have historically been very computer resource intensive. However, the CAMx user's guide states that the PiG module within CAMx is considerably faster than PiG schemes in other models, and our experience with the new algorithm indicates that this is indeed the case. Additionally, with the computer resources now available, parsimonious PiG selection is no longer critical in terms of computer resource demands.

PiG sources will be selected based on magnitude of NO_x emissions. TCEQ anticipates selecting over 300 PiG sources across the entire modeling domain, mostly large power plants. However, this number may increase or decrease as the modeling progresses.

4. Emissions Inventory

The modeling inventories being developed for modeling in BPA are largely the same as those being developed for Phase 2 of the Mid-Course Review for the HGB area. Since the modeling domain covers both the HGB and BPA areas, common inventories are being developed to serve both areas. The inventory is thus being developed for all episode days being modeled, including several days where 1-hour or 8-hour exceedances were not recorded in BPA. The discussion below will focus on those days being modeled specifically for BPA.

4.1 Base Case

The modeling emissions inventory (EI) is composed of point, area, on-road mobile, nonroad mobile, and biogenic emissions. The modeling inventory being developed for the BPA attainment demonstrations modeling will contain data from a wide variety of sources, including the 1999 periodic inventory, the 2000 annual point source inventory, data from the ARPDB, data from the TexAQS 2000 Special Inventory, link-based on-road mobile source data, and data from several special studies including a comprehensive inventory of plant species and biomass in East Texas. Day - and (in some cases) hour-specific inventories will be developed as appropriate to account for temperature and activity variation.   The entire modeling inventory is, in large part, based on the previously-built Houston Galveston Mid Course Review, Phase 1 modeling study.

No special point source emissions are available for the August 12 episode (or for the ramp-up days) because this episode day falls outside the TexAQS 2000 period. In this instance, ozone-season daily emissions extracted from the PSDB will be used for all point sources except for those reporting to the ARPDB.

4.2 Point Sources

The base case point source emission inventories will be composed of information from several databases.

For the Texas portion of the inventory, data from the point source database (PSDB) will be used. A new modeling extract will be queried from the PSDB. This inventory will be supplemented with hourly data from the acid rain program database (ARPDB) and with data obtained during the TexAQS 2000 Special Inventory.

For the August 30-September 1, 2000 episode, day and hour-specific point source emissions data that were collected for the entire TexAQS 2000 period will be used. These data were obtained by surveying the largest sources in the HGB and BPA areas to account for specific operating conditions, upsets, start-ups, and shut-downs during the specified time period. Because many of the factors that constitute the notion of rule effectiveness were directly accounted for in the survey, no rule effectiveness adjustments will be applied to emissions reported in the Special Inventory survey. The 81 potential respondents to the survey account for a large proportion of the VOC and point source emissions in the nonattainment areas. In cases where the surveys contain no information about a source or where the data are not usable, then ozone-season daily emissions - adjusted for rule-effectiveness - will be used.

Emissions from both the PSDB and the Special Inventory contain large amounts of information about specific hydrocarbons emitted by each source; however, some sources report little or no speciation of their hydrocarbon emissions. In the HGB Phase 1 modeling, any source which reported less than 75% speciation was assigned either a Texas-specific SCC-average or an EPA default speciation profile. For sources reporting 75% or more speciation, the unspeciated emissions were assumed to have the same speciation as the reported emissions. This method is a major improvement over simply assigning default speciation based on SCCs, but still leaves some less-

than-desirable results. Specifically, for any source whose emissions are less than 75% speciated, all reported speciation data is ignored. For COMA and the BPA attainment demonstration, TCEQ developed a new process which retains all speciated hydrocarbon data reported to the PSDB, regardless of how completely each point's emissions were speciated. Also new for this speciation is the exclusion of non-VOC species, as defined by EPA, from all point-source speciation profiles. These procedures are described in "Speciation of Texas Point Source VOC Emissions for Ambient Air Quality Modeling", G. Cantu, TCEQ, October 2003.

As in the extended TexAQS 2000 episode, the August 10-13, 2000 base case point source emission inventories are composed of information from several databases. The Texas portion of the August 10-13, 2000 base case point source emissions will be prepared in the same manner as those for the TexAQS 2000 episode, with the exception of the Special Inventory. This episode falls outside the TexAQS 2000 period, therefore no Special Inventory data is available for these days. The EGU emissions were updated with hourly EPA Acid Rain Program data for these episode days.

For both the August 30-September 1 and the August 12 episodes, the modeling staff will also include emissions estimated from the upset/maintenance reports submitted by companies to the local TCEQ Regional offices, (excluding events already reported in the Special Inventory).

The Louisiana Department of Environmental Quality (LDEQ) supplied to TCEQ modeling staff a copy of their 2000 point source emissions inventory in AFS format. The TCEQ modeling staff, with assistance and QA from LDEQ point source emissions staff, completed an AFS-to-ARPDB cross-reference list. This list links Louisiana acid rain boilers to their corresponding LDEQ stack identifiers. TCEQ modeling staff will replace LDEQ annual emission records in the AFS file with corresponding hourly ARPDB emissions for each hour of the episode.

For the states in the remainder of the modeling domain, beyond Texas and Louisiana, TCEQ will use the same "regional" files previously generated for the HGB Phase 1 MCR modeling. Specifically, the TCEQ obtained point source emission records in the AIRS facility subsystem (AFS) format from Environ, Inc. This data had already been prepared for near-nonattainment modeling that Environ was performing for several areas of Texas. Modeling staff reviewed the AFS file, removed Texas and Louisiana records from the file, and processed the remainder through EPS2x. TCEQ modeling staff created an AFS-to-ARPDB cross-reference list for the regional boilers larger than 750 MW capacity that are subject to EPA's Acid Rain Program. This cross-reference list links these boilers to their corresponding NEI/AFS stack identifiers. With this cross-reference file, the ozone-season daily emission records in the AFS file will be replaced with corresponding hourly ARPDB emissions for each hour of the modeled episode.

TCEQ modeling staff has been in contact with the Minerals Management Service (MMS) over the last several years to monitor the status of the 2000 Gulf-Wide Emission Inventory (GWEI). As of this writing, the data have not been provided to TCEQ, so will not be used in the current round of modeling. Therefore, the offshore point source emissions used for this modeling will be the same as those developed during Phase 1 of the HGB MCR. In Phase 1 of the HGB MCR, the 2000 offshore EI was generated by growing the 1992 MMS offshore EI, in-place, by a factor that accounted for the growth in offshore production platforms, based on a previous MMS report. Based on the recommendation of MMS staff, the entire point source offshore file was grown by 44%,

assuming that the ancillary stationary point source equipment would grow at the same rate as the number of offshore platforms.

The introduction of Mexican point sources was new to Phase 1 MCR modeling. TCEQ modeling staff converted the 1999 Big Bend Regional Aerosol and Visibility Observational (BRAVO) Study emissions inventory from IDA format to AFS format. This same Mexico emissions file was incorporated into HGB and BPA modeling runs. TCEQ modeling staff has completed a preliminary evaluation of the ERG July 2003 "1999 Mexico NEI" report and determined there were no significant differences in point source emissions. Additionally, the ERG data files have not been made available.

4.2.1 Adjusting the Point Source emissions based on ambient measurements

As was discussed extensively in the Technical Support Document of the December, 2002 HGB SIP Revision, one conclusion of the TexAQS 2000 study is that observed concentrations of certain compounds, especially light olefins, are much larger than represented in the reported emissions inventories. In the HGB Phase 1 MCR modeling, using the reported emissions resulted in a severe under-prediction bias in modeled ozone concentrations, but when a set of highly-reactive VOCs (HRVOCs) were adjusted, model performance markedly improved.

The adjustment used in the HGB Phase 1 modeling consisted of creating a second point source emissions file in the standard AFS format used by EPS2x, containing all emission points for twenty-seven large HRVOC-emitting accounts in the eight-county nonattainment area. This file was used to provide the extra HRVOC emissions necessary to make each of the 27 facilities' HRVOC emissions equal their individual NO_X emissions. The HRVOC-to-NO_X adjustment was based on the observation that airborne concentrations of light olefins measured aboard the Baylor University research aircraft frequently approximate concurrently measured concentrations of NO_Y when the aircraft passed through industrial plumes. Since the completion of HGB Phase 1 modeling, several additional studies have been conducted comparing reported inventories to ambient measurements, both airborne and ground-based. These studies generally agree that emissions of HRVOCs are significantly under-reported. Additional studies are underway, and TCEQ plans to develop refined inventory adjustments in the near future.

The approach used in HGB Phase 1 of the modeling is supported by at least one independent study conducted for the Houston Advanced Research Center by Environ (see http://www.harc.edu/harc/Projects/AirQuality/Projects/Status/Files/H6EDraftReport.pdf). This study used inverse modeling to assess various inventory components, and concluded that further modification of the inventory that was used in HGB Phase 1 was not warranted under the then-current model formulation. For HGB COMA and the BPA attainment demonstration, however, TCEQ is using a somewhat enhanced version of the adjustment used in HGB Phase 1.

The HGB Phase 1 approach has been enhanced in several ways. Most importantly, instead of adjusting all HRVOC species (which included a small adjustment of emissions of non-olefinic compounds), TCEQ has specifically targeted terminal olefins, since these are the compounds to which the aircraft instruments theoretically respond best. Second, instead of adjusting emissions at only a few selected facilities, TCEQ uses a broad-based adjustment which applies to all sources

reporting emissions of more than 10 tons/year of terminal olefins. Third, the file used to boost emissions now contains explicit hydrocarbon species appropriate to each adjusted emission point, instead of the "generic" HRVOC used in HGB Phase 1. Overall, these enhancements change the modeled reactivity slightly from Phase 1, but provide for much more flexibility in control strategy modeling.

The TCEQ plans to conduct additional studies comparing ambient concentrations of olefins to the inventory, and will work towards developing more targeted adjustments, especially now that several new automatic gas chromatographs (Auto-GCs) have been deployed in the industrial sectors of the HGB area. In addition, data collected by the Baylor aircraft over the BPA industrial area will be used as a starting point for adjusting BPA's HRVOC emissions. TCEQ will also study emissions of less-reactive VOCs to determine if and by how much these compounds are under-represented in the reported inventory. Some preliminary assessments of emissions of these compounds have already been conducted, and we will conduct sensitivity analyses of adjustments to the less-highly reactive VOC emissions. Results of these analyses will be included in the documentation for the upcoming SIP revision.

4.3 Area and Nonroad Mobile Sources

Within the four-kilometer domain, area source emissions developed for the base case by projecting the 1999 periodic emissions inventory to 2000. Emissions from nonroad sources (except for ships, airplanes, and locomotives) were generated using the NONROAD 2002a model. For several categories, local equipment populations were estimated based on surveys: lawn and garden, recreational marine, and construction activity. Emissions for ships were estimated directly from a recent survey, and emissions for locomotives and aircraft were provided by the TCEQ Emissions Inventory staff. Special treatment was applied to shipping, with ship emissions treated as pseudo-stacks spaced along the major waterways within the Galveston Bay region (as described in the December 6, 2000 SIP revision) as well as the BPA waterways.

Emissions for the remainder of Texas and for other states were obtained from Environ, who developed a 1999 inventory (based on the NEI) for modeling being conducted for the state's near-nonattainment areas. TCEQ has recently received new statewide 2000 area source emission and will incorporate these into the current round of modeling as soon as practicable. TCEQ will also apply growth to the 1999 emissions used outside of Texas to produce a true 2000 base case for area and nonroad sources.

Spatial allocation for most categories employs new surrogates developed for the HGB Phase 1 MCR modeling, including new spatial surrogates for shipping lanes.

Since TCEQ has not yet received the GWEI emissions estimates for area and nonroad sources, the agency will continue to use the same emissions as in HGB Phase I MCR.

No additional processing is required for the August 12 episode, since area and nonroad mobile sources are modeled generically with respect to daily and monthly variation.   For example, all the Thursdays in August of a given year are assumed to have identical area & nonroad mobile

source emissions. Every day of the week is already represented in the emissions being developed for the HGB COMA Mid-Course Review modeling, so we will just use the corresponding emissions files from the latter episode.

4.4 On-road Mobile Sources

In March 2002, TTI provided MOBILE6 HGB inventories for each day of the August 22-September 1 ozone episode for both the 2000 base case and a 2007 future case. As with previous development of on-road mobile source inventories for photochemical modeling purposes, TTI staff utilized travel demand model output for a specific episode year from the Houston Galveston Area Council (HGAC). For each roadway link in the eight-county HGB network, VMT and average speed estimates were developed for each hour of each episode day of interest. In order to distinguish between the differing traffic levels on the various episode days, TTI staff have developed adjustment factors based on in-use traffic survey data such as hourly traffic counts, VMT mix measurements, etc. MOBILE6 emission factor output in gram-per-mile by speed is coupled with the VMT per roadway link by hour to develop a complete on-road mobile source inventory of CO, NO_x and VOC for the entire modeling episode in the eight-county HGB nonattainment area. All emissions are adjusted a final time to account for differences between the travel-demand model and the Highway Performance Monitoring System (HPMS). In the event that the 2007 travel demand model results (which will be available during the first quarter of 2004) from HGAC are significantly different than those utilized for the existing 2007 MOBILE6 inventory, it is possible that a revised MOBILE6 inventory for 2007 will be developed by TTI and incorporated into the photochemical model by TCEQ.

In July of 2002, TTI submitted MOBILE6 link-based inventory estimates for the 3-County BPA nonattainment area. These BPA inventories also covered the August 22-September 1 ozone episode for both the 2000 base case and a 2007 future case. Only one 2007 future case inventory was developed for BPA because different speed limit scenarios were not considered. It is not anticipated that a revised 2007 future case inventory will be developed by TTI because it is not likely that the 2007 travel demand model estimates for BPA will change in the near future.

For the Texas counties within the modeling domain but outside the HGB and BPA nonattainment areas, HPMS-based VMT estimates were used by TTI to develop MOBILE6 county-wide emission inventories by roadway type for both 2000 and 2007. Due to the differing traffic profiles, inventories for each county were developed for Weekday (Monday-Thursday), Friday, Saturday, and Sunday day types. For preprocessing purposes, emissions from major roadways will be spatially allocated by appropriate roadway surrogates (e.g., interstates, state highways, etc.), while emissions from minor roadways and local streets will be allocated spatially by human population surrogates. Previously, 1999 MOBILE5-based inventories for these non-HGB counties were adjusted to MOBILE6 based on scaling factors from default runs with MOBILE5 and MOBILE6. These adjusted inventories were used in previous photochemical modeling efforts, but will be replaced by the MOBILE6 inventories developed by TTI once emissions preprocessing is completed.

In a similar fashion, emissions inventories for areas outside Texas but within the photochemical modeling domain utilized MOBILE5-based inventories which originated from EPA's 1999 National Emissions Inventory (NEI). These inventories were also adjusted with MOBIE5-6 scaling factors. As time and resources permit, these inventories will be updated with NEI MOBILE6 data.

Because the modeling episode has been expanded since HGB Phase1, additional day-specific emissions will be required. In most cases, the development of these additional days will be identical to the development of the original HGB Phase 1 episode. However, because of the time and expense required to develop day-specific emissions for the HGB and BPA regions, TCEQ plans to instead use emissions developed for the original Phase 1 episode to formulate emissions for the additional days. If days from the expanded episode match well with days in the original episode (based on temperature, day-of-week, and humidity) then TCEQ will use the emissions from the matching days in the original episode. If not, then additional adjustments will be made to provide suitable emissions for all the additional days.

Similar to what was built for 2007, a 2010 on-road inventory is also being built by TTI for TCEQ.

TCEQ staff will continue preprocessing all of the MOBILE6 on-road mobile source inventory data using the EPS2-x emissions preprocessor tool. PV-WAVE graphics software will continue to be utilized as a quality assurance tool to ensure that the modeled on-road emission levels are properly distributed both spatially and temporally.

4.5 Biogenic Sources

Over the past five years, TCEQ has commissioned several studies for the purpose of improving the biogenic emissions estimates in Texas. These studies (Yarwood et al., 1999) created a detailed vegetation map of Texas using field surveys and existing databases (Wiedinmyer et al., submitted), and developed an operational version of the Globeis biogenic emissions model (Guenther et al., 1999).

For the biogenic emissions model, TCEQ will be using the latest version of the biogenic emissions model Globeis, version 3 (Guenther et al., 2002; Yarwood et al., 2001; Yarwood et al., 2000; Guenther et al., 1999), to calculate biogenic emissions for this round of photochemical modeling. This version of Globeis includes several new features, including modules that vary the biogenic emissions according to changes in leaf area index, antecedent leaf temperatures, and drought, and an improved canopy energy balance model. TCEQ will evaluate all of these new modules before use.

Vegetation data - The land use and vegetation database used for biogenics modeling is derived from three sources:

TCEQ Texas vegetation database (Yarwood et al., 2000; Wiedinmyer et al., submitted). Based upon Texas Parks and Wildlife vegetation data, urban land use data from Braden, Collie, and

Turner Consulting, agricultural statistics from the National Agricultural Statistics Survey, and field surveys carried out during 1999;

BELD3 (Biogenic Emissions Landuse Data, version 3) (Kinnee et al., 1997). A vegetation database for the entire North American continent, prepared specifically for creating biogenic emissions inventories; and

Mexican land use and vegetation database (Mendoza-Dominguez et al., 2000). Database created by researchers at the University of Monterrey and Georgia Tech.

The land use and vegetation database is gridded according to the Lambert Conformal Projection with reference origin at 40° N, 100° W. The data are available at 4-km resolution for a domain encompassing most of the states of Texas, Louisiana, Arkansas, Oklahoma, and Mississippi. Biogenic inventories may use enhanced vegetation data for the Houston area that is being assembled during 2002-2003 by a research project involving the Texas Forest Service, the U.S. Forest Service, TCEQ, and the Houston Advanced Research Center. These data may be ready for use by March 2003, and will encompass the eight-county ozone nonattainment area, with special emphasis on Harris County. Any other high-quality land cover or vegetation data that become available may also be used.

Temperature data - TCEQ is developing temperature fields for biogenic emissions modeling by spatially interpolating temperatures measured by NWS and other appropriate weather stations throughout southeast Texas. The density of measurement stations with high-quality temperature data in southeast Texas suggests that accurate temperature fields created from interpolation. A recent paper by Vizuete et al. (2002) suggests that kriging is the best interpolation method.

Photosynthetically-active solar radiation data (PAR) - TCEQ is using a new method of deriving PAR fields for biogenic emissions modeling. In the past, TCEQ used algorithms from the BEIS2 model to estimate solar radiation from cloud cover observed at ground-based weather stations. But this method can result in inaccuracies due to the uncertainties associated with interpolation, and to the somewhat subjective nature of cloud cover observations. Therefore, TCEQ is using PAR data derived from satellite measurements whenever feasible. These data are calculated by the University of Maryland and NOAA for the Global Energy and Water Cycle Experiment (GEWEX) Continent Scale International Project (GCIP). NOAA uses a modified version of the GEWEX surface radiation budget (SRB) algorithm (version 1.1) to calculate radiation flux fields from Geostationary Operational Environmental Satellite (GOES-8) data. In addition to the GOES-8 data, the algorithm uses ancillary information from the NCEP Eta forecasting model to derive shortwave radiation fields at a regional scale. The algorithm's output is verified by comparison to ground-based solar radiation measurement stations. For further information about this method, see the GCIP/SRB web page at http://metosrv2.umd.edu/~srb/gcip/index.htm. TCEQ will be using a high resolution hourly database with spatial resolution of approximately 4 km^2.

Biogenic emissions for the August 10-13 episode were developed in a manner nearly identical to that used in the HGB COMA, using appropriate day-specific meteorological inputs. The only difference is that the photosynthetically-active solar radiation data were based upon 1 degree x 1 degree GOES satellite data, instead of the finer resolution 1/16 degree x 1/16 degree, as used in the COMA. A comparison of these two GOES datasets to broadband solar radiation data observed at

ground monitoring sites show that both GOES data sets have a high correlation with the observations, i.e., 0.95 for both the coarse and fine resolution GOES data. Both the fine and coarse GOES data were prepared for TCEQ by Dr. Rachel Pinker at the University of Maryland. The method is described in Pinker et al., 2003, Surface radiation budgets in support of the GEWEX Continental-Scale International Project (GCIP) and the GEWEX Americas Prediction Project (GAPP), including the North American Land Data Assimilation System (NLDAS) project. J. Geophys. Res. VOL. 108, NO. D22, 8844, doi:10.1029/2002JD003301.

4.6 Emissions Processing

The TCEQ has at its disposal several software packages for processing anthropogenic emissions, including SMOKE, EPS-2, Fast-EPS, and EMS-95. In this BPA base case modeling, TCEQ used a new version of EPS-2 known as EPS2x. This software is available from Environ, Inc. and executes much faster than the original EPS-2. In addition, it incorporates a new feature allowing modification of the model-ready emissions files at the county level. This feature means sensitivity runs can be conducted without re-running much of the EPS2x code. The EPS-2 family of emissions processors has several advantages over other systems including excellent reporting capabilities, stability, and ease-of-use. In addition, TCEQ staff are intimately familiar with the software and have developed numerous scripts and programs to interface with it. TCEQ will process all inventory components using EPS2x except for biogenics. Note that except for some enhancements, EPS2x is functionally equivalent to other versions of EPS-2, so it is expected to produce identical model-ready files in most cases. While TCEQ does not have sufficient resources to make a head-to-head comparison of EPS2x with the emissions processor used in previous modeling, the modeling staff exercising due diligence in ensuring that no errors have been introduced into this formulation of the emissions processor.

Biogenic emissions are being processed using the GloBEIS processing system used in the 2000 and 2002 SIP revisions, (or a new version if one becomes available).

4.7 Modeling Inventory Performance Evaluation

Aside from performing extensive quality assurance of the modeling inventory while it is being developed, TCEQ plans to perform several comparisons between the modeling inventory and ambient measurements. Because direct comparisons between emission rates and ambient air measurements are not meaningful, these comparisons are usually relative comparisons among measured compounds. For example, the NO_y/SO_2 ratio calculated from the emissions inventory can be compared to the same ratio calculated from ambient measurements. These comparisons should be made with care to ensure that the observed ambient air was actually influenced by the source of interest, and that at least one of the species in the ratio is relatively well quantified. If used judiciously, however, these comparisons can give some insight into possible shortcomings of the modeling inventory.

To date, numerous studies have compared ambient measurements with the reported emissions inventory. Researchers at several institutions including the TCEQ have compared aircraft

measurements with the reported inventory and have concluded that the reported emissions of certain highly-reactive hydrocarbons, particularly light olefins, were severely under-reported in the inventory. In addition, TCEQ staff have compared the reported emissions of light olefins with measurements made at automatic gas chromatographs (auto-GCs) in the area, and have reached similar conclusions. The Phase 1 MCR modeling relied heavily on inventory adjustments to provide a credible simulation of the original episode.

During the first half of 2003, the TCEQ will further pursue the comparison of ambient and inventoried pollutants. TCEQ plans to improve and expand several analyses begun during the Phase 1 modeling, and will extend the analysis to cover additional classes of hydrocarbons including aromatics and alkanes. HARC is also funding three studies designed to further elucidate the relationship between reported emissions and observed atmospheric quantities of ozone-forming pollutants.

The results of these studies will be used to develop improved adjustments to the modeled inventories of light olefins, and will be used to provide similar types of adjustments for other hydrocarbons emitted in significant quantities.

There is a dearth of recent ambient hydrocarbon data in the BPA area (unlike in HGB, where hydrocarbon data is routinely collected and where the vast majority of the TexAQS 2000 measurements were taken). The TCEQ has recently commissioned a series of aircraft flights in the area and plans to shortly deploy an automatic gas chromatograph in the area, and will compare the modeled inventory with measurements as soon as sufficient measurement data become available. It is unlikely that these comparisons can be completed for the first round of modeling, but results may be available for verification purposes prior to SIP adoption.

5   Meteorological Modeling

The CAMx model requires gridded meteorological inputs in order to estimate ozone transport, diffusion, and photochemistry. In order to produce such inputs, a separate meteorological model must be run, offline of the photochemical model, to generate gridded, spatially and temporally varying values of wind speed, wind direction, ambient temperature, and vertical mixing data (used to generate vertical mixing coefficients, K_v, which are in turn used by CAMx). Because of the complex coastal meteorology found along the upper Texas Gulf Coast, a prognostic or predictive meteorological model is used rather than a diagnostic wind model.

The TCEQ will be using the Penn State/National Center for Atmospheric Research (NCAR) Mesoscale Meteorological Model, version 5 (MM5) for building meteorological inputs to CAMx. MM5 is a state of the science non-hydrostatic meteorological model that has been used for a number of air quality applications across the United States. It has the following features:

- Can use three different map projections: Polar Stereographic, Lambert Conformal, and Mercator

- Can use nested grids (both one-way and two-way)

- Multiple physics options for precipitation, clouds, planetary boundary layer (PBL) depth, and atmospheric radiation

- Four-dimensional data assimilation system via nudging either to analysis or observational fields

- Portability to multiple computer platforms, including Cray supercomputers, PCs running Linux and multi-processor workstations.

5.1 August 30-September 1, 2000 Episode

Since the August 30-September 1, 2000 episode selected for BPA was previously modeled for the Houston/Galveston area, MM5-based meteorological fields have already been built for this episode. A complete description of the meteorological modeling may be found at http://www.met.tamu.edu/results/ . This site includes several reports generated by Dr John Nielsen-Gammon of Texas A&M University, who conducted the original MM5 modeling for this episode:

- *Initial Modeling of the August 2000 Houston-Galveston Ozone Episode* (Dec. 19, 2001 interim report)

- *Evaluation and Comparison of Preliminary Meteorological Modeling for the August 2000 Houston-Galveston Ozone Episode* (Feb. 5, 2002 interim report)

- *Meteorological Modeling for the August 2000 Houston-Galveston Ozone Episode: PBL Characteristics, Nudging Procedure, and Performance Evaluation* (Feb. 28, 2002 report)

- *Meteorological Modeling for the August 2000 Houston-Galveston Ozone Episode: METSTAT Statistical Evaluation and Model Runs from March-June 2002* (June 21, 2002 report)

- *Trajectory Analysis of Meteorological Simulations of the August 2000 Houston-Galveston Ozone Episode* (August 28, 2002 report)

- *Meteorological Modeling for the August 2000 Houston-Galveston Ozone Episode: Improved Data Assimilation and Statistical Evaluation* (August 30, 2002 report)
- *Application of Microwave Temperature Profiler (MTP) Data to MM5 Modeling of the August 2000 Houston-Galveston Ozone Episode* (August 30, 2002 report)

The reader is referred to these reports for a full discussion of the development of the meteorological fields for the August 30 - September 1, 2000 episode.

Environ is modeling this episode as part of a separate contract with the Houston Advanced Research Center. While these new meteorological fields are expected to be very similar to those used in the December, 2002 SIP revision, we will nonetheless compare these new meteorological

fields with the existing fields, and if appropriate may substitute the Environ-developed meteorological fields for those currently being used.

5.1.a Extended episode - August 19-September 6, 2000

For the extended TexAQS 2000 episode, new meteorological fields (including for the "core" period) were developed by Environ Corp and ATMET under contract to the Houston Advanced Research Center (HARC).   In this modeling, important physics option remained consistent with the earlier work discussed in detail by Dr. Nielsen-Gammon**.** These are:

• Atmospheric Radiation scheme - Rapid radiation transfer model (RRTM)
• Cumulus parameterization - Grell
• Explicit moisture calculations - simple ice
• Planetary Boundary Layer (PBL) algorithm - Medium Range Forecast model (MRF)

In contrast to Nielsen-Gammon's work, ATMET used the National Centers for Environmental Protection/ Oregon State University/Air Force/Hydrologic Research Lab (NOAH) land surface model to predict available soil moisture. The NOAH land surface model is initialized by EDAS re-analysis fields.

Subsequent improvements to the MM5 modeling for the extended episode include using a version of MM5 which assimilates GOES data for solar insolation (incoming radiation) and surface temperatures during the core TexAQS period of August 25th - September 1st.   This version of data assimilation has made it unnecessary to post-process MM5-predicted PBL heights, hence is favored over previous meteorological characterizations. Unfortunately, the use of GOES assimilation was limited to the original ("core") episode period and the remainder of the extended episode has not at this time been modeled using GOES. The TCEQ meteorological modeling staff are trying to acquire the software needed to prepare the remaining GOES data for input into MM5, and hope to be able to run GOES assimilation for the entire extended episode within the next few months.

5.2 August 12-13, 2000 episode

For the August 10-13, 2000 episode, TCEQ will develop meteorological fields using MM5 with the same or similar options to those used for the August 30-September1, 2000 episode. The MM5 domain is also based on the Lambert Conformal map projection defined as:

• First True Latitude (Alpha): 30°N

• Second True Latitude (Beta): 60°N

• Central Longitude (Gamma): 100°W

• Projection Origin: (100°W, 40°N)

• Spheroid: Perfect Sphere, Radius = 3670 km

The horizontal modeling domain structure consists a coarse grid continental domain and four nested subdomains: Regional Domain, East Texas Domain, Houston/Galveston-Beaumont/Port Arthur Domain, and Houston/Galveston Bay Domain. The Houston/Galveston Bay subdomain is at 1 km and may be turned off for this BPA modeling. The domain over BPA is currently nested down to 4 km, although 1km fields over BPA may be developed. Barring that, CAMx Flexinesting will be used to evaluate fine-scale ozone features. The MM5 domains are defined in Table 5-1 and shown in Figure 5-1.

Table 5-1 Definition of MM5 modeling domain

Domain	Range (km)		Number of grid cells		Cell size (km)	
	Easting	Northing	Easting	Northing	Easting	Northing
Continental	(-2808,2808)	(-2268,2268)	53	43	108	108
Regional	(-324,1620)	(-1728,216)	55	55	36	36
Eastern Texas	(-72,1116)	(-1548,-360)	100	100	12	12
HGB/BPA	(216,816)	(-1356,-816)	151	136	4	4

Figure 5-1 MM5 modeling domain
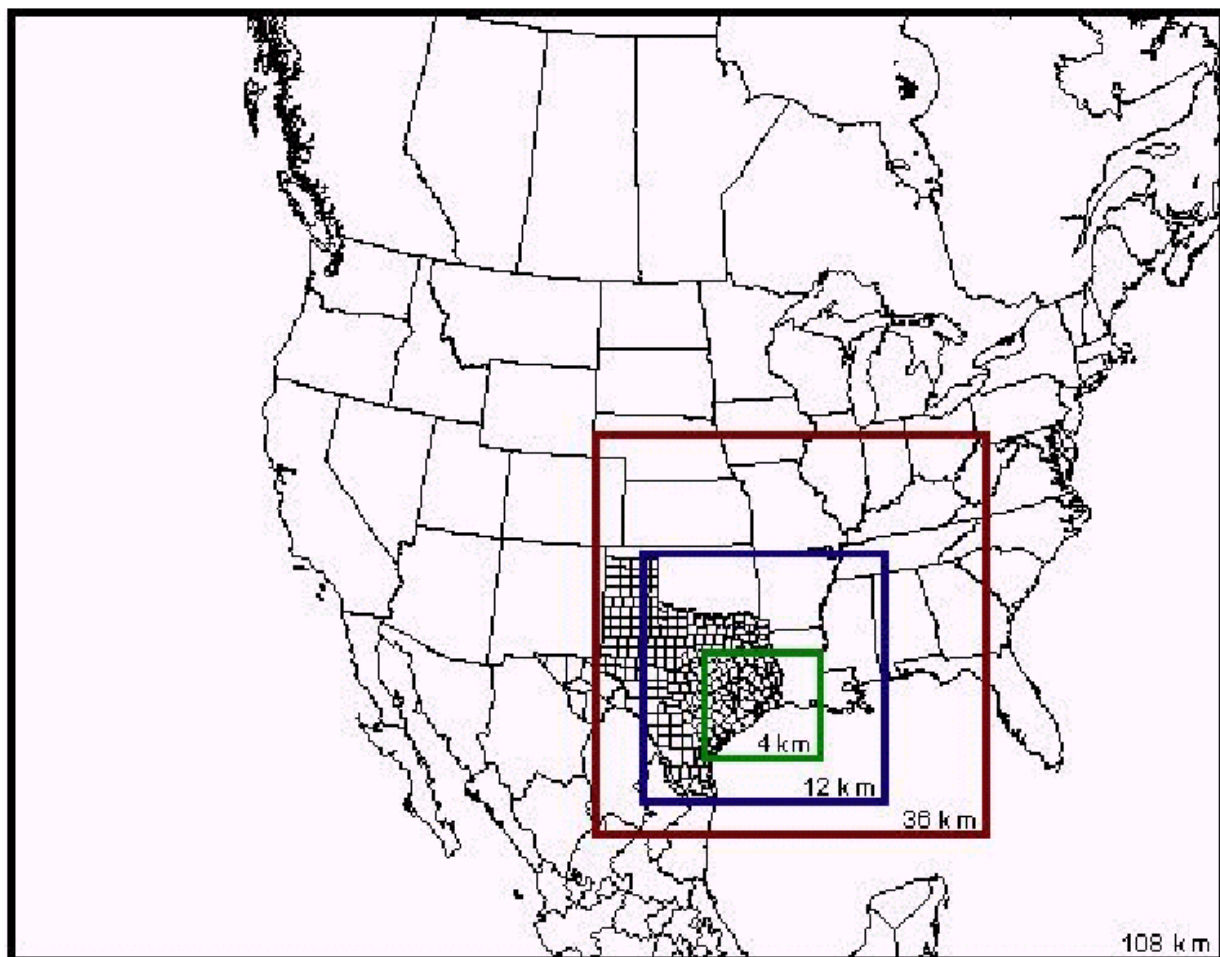
MM5 physics options to be used for the August 12, 2000 episode include:

- Atmospheric Radiation scheme: Rapid Radiation Transfer Model (RRTM)
- Cumulus Parameterization: Grell
- Explicit Moisture: Simple Ice
- Planetary boundary layer scheme: Medium Range Forecast Model (MRF)

Although sophisticated land surface interaction models were used by Texas A&M University to build the August 30-September 1, 2000 episode, that approach is currently not contemplated for the August 12, 2000 episode. The August 30-September 1, 2000 episode also used a technique that dried out the soil moisture as the episode progressed, in order to account for the hot, dry conditions (ambient temperatures during that episode were consistently in the high 90s/low 100s with no rain occurring until the end of that episode). Initially, TCEQ does not anticipate doing likewise for the August 12, 2000 episode, unless MM5 performance requires it.

5.3 Meteorological Performance Evaluation

The TCEQ believes that since ozone-conducive meteorology is a critical component of the photochemical modeling process, it is imperative that there be a substantial degree of confidence in the gridded meteorological fields. Therefore, in 2001, the TCEQ contracted with Environ, International to develop a software tool, called METSTAT, that is used to evaluate predicted vs observed meteorological parameters of wind speed, wind direction, ambient temperature, and humidity. The evaluation looks at time series traces and bar graphs using the various metrics such as bias, gross error, Root Mean Square Error (RMSE), and Index of Agreement (IOA). The statistical benchmarks or performance targets are listed in Table 5-2. A complete discussion of how these benchmarks were developed may be found in the report *Enhanced Meteorological Modeling and Performance Evaluation for Two Texas Ozone Episodes* (August 2001).

Table 5-2 Meteorological Modeling Benchmarks

Metric	Benchmark
Wind speed total RMSE	2.0 m/s
Wind speed IOA	0.6
Wind direction gross error	20 degrees
Temperature bias	± 0.5 K
Temperature gross error	2.0 K
Temperature IOA	0.7
Humidity bias	± 1.0 g/kg
Humidity gross error	2 g/kg

Humidity IOA	0.7

TCEQ will use these statistical tools and graphical representations of the MM5 output to guide evaluation of when the meteorological field predictions are optimal. When these meteorological performance is acceptable, the fields must be converted into a form that can be readily used by the CAMx photochemical model.

5.4 MM5 to CAMX Post-processing

The preparation of meteorological fields for the CAMx model requires post-processing by a program called MM5CAMx. MM5CAMX was written by ENVIRON. Horizontal interpolation of MM5 variables is unnecessary since the MM5 and CAMx grids utilized the same Lambert-Conformal projection. Vertical interpolation will be minimized by defining matching sigma levels in the lowest ten layers. For the purposes of air quality modeling, the extent of vertical mixing is of great importance. Using the MRF parameterization scheme, which was part of the MM5 driver configuration developed by Dr. Nielsen-Gammon for the August 25-September 1, 2000 episode, a predicted planetary boundary layer (PBL) height is calculated by MM5.

An alternative PBL scheme, called Gayno-Seaman (not proposed for this study) calculates turbulent kinetic energy (TKE) as well. The post-processing program MM5CAMx does the required interpolation of meteorological variables from MM5 to CAMx grids, and equally importantly, uses information about PBL height or TKE to calculate the vertical diffusivities needed by CAMx.

One of the inherent difficulties in evaluating the PBL performance of MM5, and how it, in turn, generates vertical diffusivities in MM5CAMX is the fact that there were no radar profilers or sodars in BPA during TexAQS 2000.

6 Model Performance Issues

6.1 Quality Assurance Testing of Inputs

At each step prior to conducting base case simulations, the input fields will be reviewed for consistency and obvious errors. Graphical and statistical techniques will be used where appropriate to quality assure the data input to CAMx. This includes an analysis of the results from preprocessor programs.

6.1.1 Meteorology

Wind vectors, temperature, and the vertical exchange K_v for each grid square will be plotted for selected hours and analyzed to determine if the data are appropriate, consistent, and correctly distributed. Meteorological performance evaluation techniques will also be used as a part of the meteorological quality assurance.

6.1.2 Emissions Inventory

Daily emissions inventory summary graphics displaying grid cell emission densities for the various source types will be developed for each pollutant to determine if the emissions appear to be appropriate, consistent and correctly distributed.

6.1.3 Air Quality

For initial conditions air quality data for each grid square for selected hours will be plotted and analyzed to determine if the data are appropriate, consistent, and correctly distributed.

6.1.4 QA/QC Plan

The modeling staff conducts extensive Quality Assurance/Quality Control (QA/QC) activities when developing modeling inputs, running the model, and analyzing and interpreting the output. TCEQ has developed a number of innovative and highly effective QA/QC tools that are employed at key steps of the modeling process. Appendix C provides a detailed QA/QC plan developed by the modeling staff to be used during modeling for the Mid-Course Review.

6.2 Diagnostic Evaluation and Testing

Diagnostic evaluation is an assessment of a model's ability, when functioning as a whole, to predict specific details or processes occurring during a photochemical episode. The events and tests are specifically chosen to challenge the science in the model. Specific focus is on detailed examination of how well individual components of the model simulate actual atmospheric processes.

Observational and model derived data are not completely adequate to describe meteorological and air quality fields in all areas of a modeling domain. Therefore, input files for photochemical grid models describing these fields are, at best, estimates. Diagnostic evaluation of simulation results may be used to test the adequacy of input data files and provide a basis for improved estimates. The evaluation is based on comparisons between observed and simulated air quality and comparing areas of poor agreement with uncertainties in the input data. Where such areas of uncertainty are found to exist, input fields may be modified, through an iterative procedure, to improve simulation results. However, such modifications must be based on sound scientific principles and not conflict with observed data.

6.3 Sensitivity Testing with the Base Case Simulations

Sensitivity tests are designed to check responses of the base case simulation to the plausible variability in the various model inputs. That is, given a possible change to some input parameter (e.g., doubling mobile emissions), the change in base case ozone production is determined. The results of these tests indicate the sensitivity of the model to various inputs and provide a guide by which modeling inputs may be reasonably adjusted to achieve acceptable model performance, as well as point out which inputs must be scrutinized most closely.

The following basic tests will be performed to determine sensitivity to various model input parameters:

- Wind speed modification - Note that wind-speed modifications, although recommended in EPA Guidance, must be approached carefully, since simply changing the wind speed affects the conservation of mass, momentum, and energy in the wind fields. Any alterations in wind speed will be chosen in such a way as to suggest possible ways to improve model performance.

- Alternative boundary conditions - As noted in Section 3.6.5, boundary conditions may be playing an important role in peak ozone in BPA. This may be even more true when evaluating 8-hour concentrations. Additional sensitivity runs may be conducted to assess the range of effects that boundary conditions have on BPA. Runs will also be conducted to determine the sensitivity of the model to the top boundary conditions.

- Alternative emissions inventory assumptions - Several emissions sensitivities will be conducted to determine how the model results change as a result of modifying components of the emission inventory. The modifications will be based on the estimated uncertainty in the emission components as well as on comparisons of the modeling inventory with ambient measurements. See Section 4.2.1.

- Alternative vertical mixing - EPA Guidance has historically recommended sensitivity testing to determine the model's response to perturbations in mixing height. Newer models, including CAMx, use instead a vertical mixing coefficient commonly known as KV. Because vertical mixing is critical to the success of the modeling application, TCEQ intends to perform additional sensitivity testing of this key parameter to assure that the model adequately replicates the actual mixing.

The exact nature of the alterations to model inputs will be determined after analyzing the performance of the base case. The results of each analysis will be compared to the base case to determine the change in ozone produced by these changes in inputs.

In addition to the tests described in this section, tracer simulations will be conducted to determine the contributions of initial and boundary conditions to the area of interest. These tracer simulations were described above in the section on boundary and initial conditions.

7 Model Performance Evaluation

The performance of CAMx for the base case will be evaluated to determine whether the model is adequately simulating the formation of ozone. CAMx must show reasonable performance for each base case episode before the meteorological data for the episode are used with the future year emissions inventory to determine future control strategies.

7.1 Performance Measures

Since the first day or two (ramp-up days) of a modeling episode are initializing days during which exceedances were not recorded, performance measures will be applied to modeling results subsequent to the episode ramp-up days. These measures include qualitative (graphical) and quantitative (statistical) evaluations.

CAMx predicts a volumetric one-hour average over the whole grid cell. Monitoring data provide a measure of air quality at a specific point in space. To provide an accurate comparison with model predictions, the monitoring data would have to be transformed into volumetric one-hour averages over the same grid cells used in CAMx. However, monitoring networks are not dense enough to provide this information even for the most intensive studies that have been performed. Thus, comparison between the CAMx volumetric predictions and the monitored point measurements are the only recourse. This can provide insight into model prediction trends, but does not provide precise measures of model performance. A detailed description of specific comparisons is found in *Improvement of Procedures for Evaluating Photochemical Models*, by Tesche, California Air Resources Board. Additional information on specific procedures is found in the UAM modeling guidelines.

7.1.1 Graphical Methods

Graphical displays comparing predicted to observed concentrations can provide information on model performance. The following techniques will be used for days subsequent to the ramp-up day(s):

♦ Time-Series Plots: For each monitoring station in the domain and for each hour in the episode, the predicted concentration will be compared with the monitored concentration. This will determine whether the model can predict the peak concentrations and if the timing of ozone generation in the model agrees with that found with the monitoring. Because modeled concentrations are compared with data from monitoring sites, which are specific points in space, it should not be expected that agreement would be excellent.

♦ Surface-Level Isopleths: For selected hours, surface-level isopleths (lines of equal concentration) will be drawn. This shows how the model is predicting the extent, location, and magnitude of ozone formation. This information can be compared to monitoring results.

♦ Scatter Plots: Scatter plots of predictions compared to observations depict the extent of bias in the ensemble of hourly data pairs. Systematic positioning of data points around the perfect correlation line indicates bias. The distribution of points over the area is an indication of error. This procedure also indicates outlier pairs.

♦ Animations: Model output will be rendered into an animated sequence showing the formation and transport of ozone (and its precursors) throughout each episode. These animations will be compared to the conceptual models developed for the respective episodes to assure that the model replicates TCEQ's understanding of the process. If the animation differs fundamentally from the conceptual model, then both the model formulation and the conceptual model will be reviewed and revised as appropriate.

7.1.2 Statistical Methods

These methods can provide a quantitative measure of model performance. The results of these methods must be considered carefully, especially in cases where there are not a large number of monitors:

♦ Unpaired Highest-Prediction (Peak Domain Maximum) Test: This measure compares the difference between the highest observed value and the highest predicted value found over all hours and over all monitoring stations.

♦ Normalized Bias Test: This test measures the model's ability to replicate observed patterns. Since there are many time periods when relatively low levels of ozone are predicted and statistics from these periods are not very meaningful, this test will be limited to pairs where the observed concentration is greater than 0.060 ppm. This threshold is notably above the naturally occurring ozone background value of 0.040 ppm.

♦ Gross Error Test: This test will compare the differences between all pairs of predictions and observations that are greater than 0.060 ppm. This is a measure of model precision.

7.2 Assessing Model Performance Results

All performance evaluation tests listed above will be performed for each base case for days subsequent to the ramp-up day(s). The goals for the results of the statistical tests are the following:

Unpaired peak prediction: ± 15 - 20%
Normalized bias: ± 5 - 15%
Gross error: + 30 - 35%

If the statistical measures for a base case do not fall into these ranges or if the graphical analysis indicates poor performance, the input data for the base case will be carefully analyzed along with the results of the sensitivity tests. If it appears appropriate, certain sensitive inputs developed with uncertain data may be modified to yield better model performance. Any modifications to input data will be coordinated with the Photochemical Modeling Technical Review Committee and the EPA, Region 6 Office. This process will be approached very carefully because good model performance must be obtained for the correct reasons, and must not be considered an end goal in itself.

7.3 Model Performance for Ozone Precursor Species

Unlike the HGB region, the BPA region has little ambient hydrocarbon data which can be compared with model predictions. Some 24-hour canister data was collected during the two modeled episodes, but the usefulness of this data is questionable for purposes of model evaluation. Routinely collected measurements of CO, however, can provide significant insight into model behavior.

While performance analysis of non-ozone species is very valuable and provides great insight into the model's workings, it is not appropriate to base model performance evaluations directly on these species. First and foremost, CAMx (as well as similar models) is optimized to predict ozone, not NO, NO_2, PAN, or any other CB-IV species besides ozone. Second, many emissions of primary

species are on a scale much smaller than the model's finest spatial resolution. Ozone, on the other hand, is a secondary pollutant and its concentration normally is expected to remain relatively constant across areas of a few to several kilometers in width (one reason why short-term ozone peaks are difficult for the model to replicate). Finally, no statistical performance evaluation criteria are available from EPA for non-ozone species, so only graphical performance analysis techniques can be applied.

Nonetheless, TCEQ will carefully consider how well the model replicates the spatial and temporal distributions of all CB-IV species for which comparable measurements are available. Major discrepancies involving these species will be investigated to seek causes in the model formulation.

8   Future Year and Future Case Inventory Development

8.1 Future years

In light of the BPA area's bump-up, under the older 1-hour standard, to either serious or severe, EPA proposed that a 2005 attainment date be used. EPA's rationale for using this date is beyond the scope of this protocol.   Based on currently available information, TCEQ proposes to use 2007 and 2010 as BPA's future modeling years for the following reasons:

- This BPA SIP revision will be addressing three primary issues: (1) modeling analysis demonstrating continued attainment of the 1-hour standard, based on the original 2007 attainment date; (2) a 2005 Weight of Evidence-based 1-hour demonstration ; and (3) a 2010 case to assess the anticipated level of reductions needed to meet the 8-hour ozone standard.

- The 2001 BPA attainment demonstration SIP revision (since disapproved by EPA) used a 2007 attainment date because transport of ozone and precursors from HGB affects maximum ozone concentrations in BPA. It is therefore still prudent to assess the effect of HGB controls upon BPA when HGB is required to attain the 1-hour standard.

- EPA's draft 8-hour implementation guidance indicated that 8-hour nonattainment areas with design values of .085-0.092 ppm should be classified as marginal, with a 2007 attainment date. The range for moderate areas is 0.092 - 0.107 ppb. Moderate areas have until 2010 to attain. Similarly, serious areas' design values range from 0.107 - 0.120 ppm and their attainment date is 2013.

- For 2001-03, BPA's 8-hour design value is 91 ppb (0.091 ppm). The HGB area's design value is 102 ppb. For 2000-02, BPA's design value was 90 ppb and HGB's was 107. Under EPA's proposed classification system, for either set of years, BPA would be marginal. Depending on which 3-year set is used, HGB would be either moderate or serious. Given that HGB will not have to attain until possibly as late as 2013, and the fact that part of BPA's ability to attain the 8-hour standard is tied to HGB, it is logical to assume that BPA could not attain by a 2007 attainment date.

- With the advent of the 1-hour bump-up, BPA's major source thresholds and offset ratios will be more stringent than that required of an 8-hour marginal or moderate area (major source thresholds and offset ratios are the same for either the 1-hour or 8-hour standard). Section 182(b)(3) of the Federal Clean Air Act states: *The Administrator shall grant the request of any State to reclassify a nonattainment area in that State in accordance with table 1 of subsection (a) to a higher classification. The Administrator shall publish a notice in the Federal Register of any such request and of action by the Administrator granting the request.* Therefore, BPA may petition to be classified higher in order to have more time to reach attainment. A request for attainment classification of moderate or marginal would not substantively affect BPA's point source nonattainment review requirements.

- Therefore, for the 8-hour standard, TCEQ plans to use a 2010 future year for BPA in order to (1) provide more time to attain and (2) align BPA more closely with HGB (especially should HGB be designated moderate).

- This BPA SIP revision's 8-hour component will provide an initial focus on BPA's 2010 8-hour ozone modeling, but not necessarily an 8-hour attainment demonstration.

- Again, for addressing the 1-hour ozone standard with a 2005 attainment year, TCEQ will address this by Weight of Evidence. A more complete discussion of that WoE component would be more fully described in an update to this modeling protocol.

8.2 Future Case Inventory Development

After the base case CAMx modeling has demonstrated that it can reproduce ozone and meet EPA performance criteria, the base case inventory must be grown out to the future/attainment year. Due to the nature of the modeling exercise, TCEQ will build inventories for 2007 and 2010. The discussion here does not include changes in the inventory due to controls or reductions. Changes in the future case due to controls is discussed in Section 9.

Point Sources

Phase 1 MCR modeling of the Houston/Galveston/Brazoria area included essentially zero growth in the nonattainment counties, due to emission caps, and assumed only EGU growth in the attainment counties of East Texas, via review of permit applications for large NOx sources that are expected to be operating by 2007. This approach will be used for the BPA future year point source growth as well. TCEQ modeling staff, emissions inventory staff and permitting staff will work together to obtain data on emission trends and emission caps. Emission inventory staff are currently in the process of analyzing VOC and NOx emission changes, in order to try to predict emissions for 2007. From these data, staff will derive emissions "projection factors" for the nonattainment areas and the attainment areas. Modeling staff will update the list of modeled "newly-permitted" large NOX sources to include the latest available dates of construction or destruction. Banked emissions (ERCs and DERCs) expected to be used in/by 2007 will be incorporated into the 2007 projection. Emissions Cap and Trade staff of the TCEQ compiled a database of sources that are subject to the HGB emissions cap. Their database is compiled for the nominal 90% reductions ESAD case. So, for

final modeling of Phase 1 of the MCR, modeling staff estimated the alternate ESAD (nominal 80% NOx reductions) capped emissions from the Cap and Trade database. Since modelers recognize that the 80% NOX ESAD reductions were approximate, modeling staff will work with the Cap and Trade staff to refine the reductions applied. These data will be used to "control" emission to their 2007 level.

Discussions with State of Louisiana SIP staff indicated that no additional controls, beyond what TCEQ staff applied to the Baton Rouge area in Phase 1 MCR modeling, are expected in Louisiana by 2007. Similarly, the growth and controls applied for the Region (outside of Texas and Louisiana), in Phase 1 MCR modeling, are assumed to be adequate for this next phase. Discussions with MMS staff concluded that it may be appropriate to grow the offshore platforms and ancillary equipment by approximately another 44%, to account for the growth from 2000 to 2007, but would be very inaccurate to perform this growth in place. The trend in new offshore equipment in Texas and Louisiana is to move much farther offshore. No accurate growth projections are available, but trends indicate such. Unless better information regarding future emissions can be obtained from MMS, TCEQ staff may perform sensitivity analyses on distance from-shore to determine if the impact on HGB of sources located far out in the Gulf of Mexico (beyond, say, 50 or 100 miles).

Area and Nonroad Mobile Sources

Activity growth for area and nonroad mobile sources will be performed on a case-by-case basis, using the best available projections. Local data from regional planning bodies and data obtained from industry groups will be utilized whenever possible. In cases where no local data are available, TCEQ will use population and/or econometric forecasts such as EGAS as appropriate. For nonroad categories, the NONROAD model will be used to project emissions into the future since it accounts for both growth and federal controls on nonroad sources.

On-road Mobile Sources

The 2007 and 2010 on-road mobile source EI for the BPA nonattainment area will be developed by TTI staff in a manner consistent with that described in for the base case inventory. The main differences will be that travel demand model output and MOBILE6 runs for 2007 and 2010 will be used instead of those for the base year. The 2007 and 2010 travel demand model runs will be based on best available projections of future population growth, demographic patterns, and roadway network changes. The MOBILE6 runs for 2007 and 2010 will utilize the same meteorological inputs as the base year (temperatures, humidity, etc.), but other inputs will change as appropriate. Projecting into the future, it is expected that both the human and vehicle population in the BPA (as well as HGB) area will increase, thus causing an increase in daily VMT on the roadway network. However, typical turnover effects will yield a vehicle fleet more heavily populated with newer "cleaner" vehicles as opposed to older "dirtier" ones. As with the base case, emissions from the original episode will be used to produce emissions for the expanded episode days.

Biogenics

Biogenic emissions will be assumed to remain unchanged in the future, although urban development does modify the amount, location, and type of vegetation over time. TCEQ plans to

investigate the use of projected land-use data to estimate attainment-year biogenic emissions in future modeling applications.

9 Control Strategy Testing and Attainment Demonstration

Once the base case modeling demonstrates that the model is able to accurately simulate ozone production over the episodes, and the future case inventories are completed, control strategy testing will commence. The first control case with the future base inventory will also include all control programs that were not in place at the time of the episodes, but will be by 2007 and 2010. These measures will include:

Stationary sources

Three-county BPA nonattainment area

•   Chapter 117 rules adopted in 2000 - these are the point source NOx rules affecting boilers, heaters, utility boilers, turbines, lean burn gas-fired internal combustion engines and rich burn gas-fired in rich-burn internal combustion engines

Eight-county Houston/Galveston/Brazoria nonattainment area:

•   Point source NOx reductions (80%) - Current Chapter 117 rules
•   Chapter 115 HRVOC rules affecting:
•   Cooling towers
•   Vent gas control and flares
•   Fugitive emissions leak detection and repair (LDAR)
•   Site-wide HRVOC caps (currently proposed rule for HGB)

Statewide reductions

•   Texas electric generating units (NOx) due to Senate Bill 7
•   Agreed orders with: Alcoa-Rockdale (NOx), TXU units in the DFW and North East Texas area (NOx), AEP units in North East Texas (NOx), and Eastman Chemical-Longview (NOx and VOC).

This modeling will also include wide-spread NOx reductions due to EPA NOx SIP call (NOx SIP call states only).

On-road mobile sources

Houston/Galveston/Brazoria 8-county area

- Inspection & Maintenance - September 2001 HGB SIP revision - Two-speed idle or ASM-2 inspection/maintenance program for Harris, Brazoria, Galveston, Fort Bend, and Montgomery counties only
- Cleaner diesel fuel
- VMEP
- Speed limit reduction (65-60)
- Gas-fired water heaters, small boilers, and process heaters
- Stationary diesel engines

Central and east Texas counties and BPA :

- Clean-burning gasoline (RVP 7.8)
- FMVCP
- NLEV standards
- Federal low sulfur gasoline
- Tier II vehicle emission standards
- Heavy-duty diesel standards

Although additional on-road controls (I&M) may be imposed in the Austin Early Action Compact area by 2007, that strategy is not included in this modeling.

Nonroad Mobile Sources

Houston/Galveston/Brazoria 8-county area

- RFG fuel standards
  Low emission diesel
  California spark ignition engine rule

Statewide

- EPA Heavy Duty Diesel Engine rule

Central and east Texas counties (excluding HGB and BPA nonattainment counties):

- Clean-burning gasoline (RVP 7.8)

Central and east Texas counties plus HGB and BPA nonattainment counties:

- Locomotive standards
- Compression ignition standards for vehicles and equipment
- Spark ignition standards for vehicles and equipment
- Commercial marine vessel standards
- Recreational marine standards
- Heavy duty diesel standards

Nonroad emission reductions due to the Texas Emissions Reductions Program (TERP) have not been quantified.

Area Sources (statewide)

•   Low NOx standards for new water heaters and furnaces

        When the future case, plus controls, is simulated in CAMx, the 2007 model results will be compared to the level of the 1-hour standard, which is 125 ppb, as well as the new 8-hour standard, which is 85 ppb. The 8-hour results will also be calculated for 2010, which is anticipated to be BPA's 8-hour attainment year. However, EPA's draft 8-hour attainment demonstration modeling guidance indicates that the model results should be used in a relative manner. So, both 2007 and 2010 modeling results will be used to estimate future 8-hour (and 1-hour) design values via the Relative Reduction Factor (RRF)/Future Design Value approach. In short, this approach will multiply the current design values for BPA-area monitors times the ratio of the future/control case predicted ozone to the base case predicted ozone for each monitoring site. The objective is for all monitors to show future design values below 85 ppb.

        Should 2010 Future Design Value calculations equal or exceed 85 ppb, TCEQ will run emission reduction sensitivities to estimate the anticipated range of reductions of NOx and/or VOC needed in BPA to attain the 8-hour standard. However, this exercise will not include development and modeling of any additional rules needed to meet the 8-hour standard. If necessary, the BPA 8-hour attainment demonstration will be done in a follow-on SIP revision.

        TCEQ may also employ Weight of Evidence (WoE) techniques to bolster the attainment demonstration. These may include, but not be limited to, emission trends, air quality trends, advanced modeling metrics, and meteorological analyses.

10   Procedures to Archive and Document Study Results

        EPA recommends that certain types of documentation be provided along with a photochemical modeling attainment demonstration. The TCEQ is committed to supplying the material needed to ensure that the technical support for any SIP revision is understood by all involved parties. To that purpose, the TCEQ will document the following items in conjunction with the attainment demonstration:

●   Modeling Protocol – Establishes the scope of the analysis and encourages stakeholder participation in both the study development and the study itself.

●   Emissions Inventory Final Report – Summarizes the development of the model-ready emissions estimates database. This report will contain tabular and graphical summaries of the data for both base and future years.

- Air Quality/Meteorological Input Final Report – Summarizes the development of the meteorological and other needed model input fields. This report will contain tabular and graphical summaries of the relevant data.

- Model Performance Evaluation Report – As discussed in Section 7, an assessment of the suitability of the model to support emissions control policy will be assessed. The findings of that analysis will be discussed comprehensively in the model performance evaluation report. Also, as discussed in Section 6, several diagnostic analyses are planned to determine whether the photochemical modeling results are physically sound. The results from these analyses will be included as part of the performance evaluation report.

- Description of the Attainment Demonstration Strategy – The documentation (likely as part of a final report) will outline the specific control measures which embody the attainment demonstration plan. A description of the modeling, that suggests attainment will be achieved in a future year, will be provided. If any "weight-of-evidence" arguments are used to supplement the findings of the air quality modeling, a description of the techniques used and a summary of the findings will also be documented.

- Graphical depictions of the modeling results – These will include ozone isopleth plots, difference isopleth plots, and ozone animation sequences, will be produced to aid in sharing model results with EPA, the TCEQ management, and stakeholders.

- External Review – The TCEQ will document the review procedures (internal and external) employed in the project. This review will include instructions for interested external parties to access the study database, including software utilized as part of the technical analyses.

Additionally, the TCEQ will archive all documentation and modeling input/output files generated as part of the BPA CAMx modeling. Mr. James Red of the TCEQ will be responsible for these products and may be reached by telephone at (512) 239-1465 for information regarding data access or project documentation.